



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:47 PM GMT

PDB ID : 3S6K  
Title : Crystal structure of xcNAGS  
Authors : Shi, D.; Li, Y.; Cabrera-Luque, J.; Jin, Z.; Yu, X.; Allewell, N.M.; Tuchman, M.  
Deposited on : 2011-05-25  
Resolution : 2.80 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

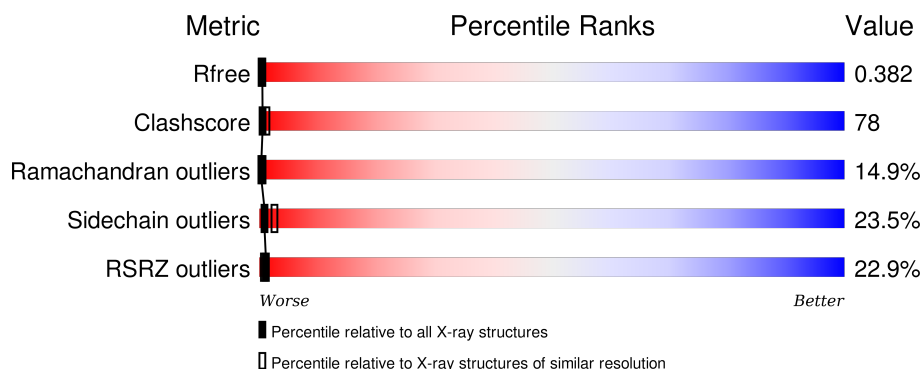
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	467	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3407 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 Acetylglutamate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	Se	0	0	0
			3407	2159	593	647	3	5			

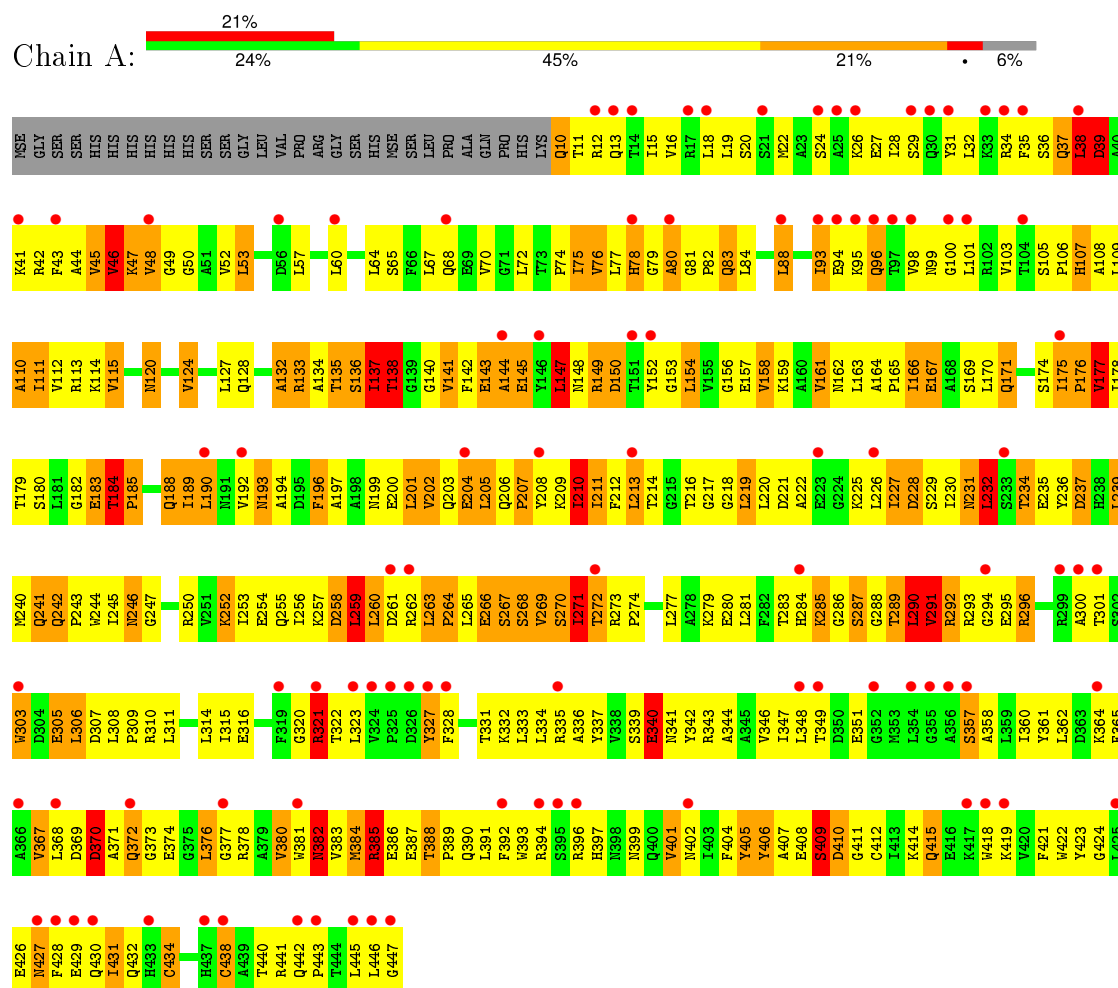
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP Q4UVI7
A	-18	GLY	-	EXPRESSION TAG	UNP Q4UVI7
A	-17	SER	-	EXPRESSION TAG	UNP Q4UVI7
A	-16	SER	-	EXPRESSION TAG	UNP Q4UVI7
A	-15	HIS	-	EXPRESSION TAG	UNP Q4UVI7
A	-14	HIS	-	EXPRESSION TAG	UNP Q4UVI7
A	-13	HIS	-	EXPRESSION TAG	UNP Q4UVI7
A	-12	HIS	-	EXPRESSION TAG	UNP Q4UVI7
A	-11	HIS	-	EXPRESSION TAG	UNP Q4UVI7
A	-10	HIS	-	EXPRESSION TAG	UNP Q4UVI7
A	-9	SER	-	EXPRESSION TAG	UNP Q4UVI7
A	-8	SER	-	EXPRESSION TAG	UNP Q4UVI7
A	-7	GLY	-	EXPRESSION TAG	UNP Q4UVI7
A	-6	LEU	-	EXPRESSION TAG	UNP Q4UVI7
A	-5	VAL	-	EXPRESSION TAG	UNP Q4UVI7
A	-4	PRO	-	EXPRESSION TAG	UNP Q4UVI7
A	-3	ARG	-	EXPRESSION TAG	UNP Q4UVI7
A	-2	GLY	-	EXPRESSION TAG	UNP Q4UVI7
A	-1	SER	-	EXPRESSION TAG	UNP Q4UVI7
A	0	HIS	-	EXPRESSION TAG	UNP Q4UVI7

### 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: Acetylglutamate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6 <sub>2</sub> 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.23 Å   133.23 Å   191.36 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	46.07 – 2.80 46.07 – 2.80	Depositor EDS
% Data completeness (in resolution range)	71.5 (46.07-2.80) 71.3 (46.07-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.321 , 0.388 0.325 , 0.382	Depositor DCC
$R_{free}$ test set	994 reflections (5.72%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.2	Xtriage
Anisotropy	0.873	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 138.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	6 of 19904 reflections (0.030%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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	A	0.51	1/3461 (0.0%)	0.77	4/4684 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLU	CG-CD	6.74	1.62	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	LEU	CA-CB-CG	6.72	130.75	115.30
1	A	138	THR	N-CA-C	6.00	127.19	111.00
1	A	242	GLN	C-N-CD	-5.84	107.75	120.60
1	A	232	LEU	CA-CB-CG	-5.49	102.68	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ILE	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3407	0	3438	535	0
All	All	3407	0	3438	535	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 78.

All (535) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TYR:HB2	1:A:346:VAL:HG22	1.26	1.16
1:A:210:ILE:HD11	1:A:212:PHE:HE1	1.05	1.15
1:A:67:LEU:HD12	1:A:74:PRO:HG3	1.26	1.10
1:A:334:LEU:HD13	1:A:360:ILE:HD13	1.19	1.10
1:A:209:LYS:O	1:A:210:ILE:HG22	1.50	1.10
1:A:269:VAL:HG12	1:A:270:SER:H	1.13	1.10
1:A:178:ILE:HG22	1:A:179:THR:H	1.01	1.09
1:A:357:SER:HB2	1:A:358:ALA:HA	1.16	1.09
1:A:124:VAL:HG11	1:A:136:SER:H	1.14	1.05
1:A:211:ILE:HD11	1:A:213:LEU:HD12	1.38	1.05
1:A:188:GLN:HE21	1:A:189:ILE:N	1.53	1.05
1:A:190:LEU:HD22	1:A:190:LEU:H	1.22	1.04
1:A:137:ILE:HG13	1:A:137:ILE:O	1.58	1.02
1:A:290:LEU:O	1:A:291:VAL:HG12	1.58	1.02
1:A:174:SER:O	1:A:176:PRO:HD3	1.59	1.01
1:A:292:ARG:HG2	1:A:292:ARG:HH11	1.21	1.01
1:A:210:ILE:HD11	1:A:212:PHE:CE1	1.95	1.01
1:A:256:ILE:HG23	1:A:269:VAL:HG21	1.40	1.00
1:A:357:SER:CB	1:A:358:ALA:HA	1.92	0.99
1:A:290:LEU:HD13	1:A:291:VAL:H	1.28	0.98
1:A:213:LEU:HD23	1:A:274:PRO:HG3	1.46	0.98
1:A:269:VAL:HG12	1:A:270:SER:N	1.78	0.98
1:A:84:LEU:HD21	1:A:88:LEU:HD12	1.47	0.97
1:A:178:ILE:HG22	1:A:179:THR:N	1.80	0.95
1:A:105:SER:O	1:A:108:ALA:HB3	1.67	0.93
1:A:441:ARG:HH11	1:A:441:ARG:HG3	1.29	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:O	1:A:260:LEU:HD12	1.70	0.91
1:A:111:ILE:O	1:A:115:VAL:HG23	1.70	0.90
1:A:109:LEU:H	1:A:109:LEU:HD12	1.36	0.90
1:A:47:LYS:O	1:A:47:LYS:HG3	1.67	0.90
1:A:133:ARG:O	1:A:174:SER:HB3	1.71	0.89
1:A:211:ILE:CD1	1:A:213:LEU:HD12	2.04	0.88
1:A:321:ARG:H	1:A:321:ARG:HD2	1.38	0.88
1:A:213:LEU:HD11	1:A:277:LEU:HD12	1.55	0.88
1:A:334:LEU:HD13	1:A:360:ILE:CD1	2.03	0.88
1:A:269:VAL:CG1	1:A:270:SER:H	1.84	0.87
1:A:12:ARG:HA	1:A:15:ILE:HG22	1.53	0.87
1:A:292:ARG:CG	1:A:292:ARG:HH11	1.87	0.87
1:A:77:LEU:HD12	1:A:201:LEU:HD23	1.56	0.86
1:A:270:SER:O	1:A:272:THR:HG22	1.75	0.86
1:A:392:PHE:HB3	1:A:438:CYS:SG	2.16	0.86
1:A:211:ILE:HD12	1:A:212:PHE:N	1.91	0.85
1:A:127:LEU:HD22	1:A:175:ILE:HD11	1.59	0.85
1:A:188:GLN:HE21	1:A:189:ILE:H	1.19	0.85
1:A:341:ASN:HD22	1:A:343:ARG:HE	1.24	0.84
1:A:391:LEU:HB3	1:A:423:TYR:HB3	1.59	0.84
1:A:202:VAL:HG22	1:A:207:PRO:HG2	1.59	0.84
1:A:311:LEU:O	1:A:315:ILE:HG13	1.77	0.84
1:A:178:ILE:CG2	1:A:179:THR:H	1.89	0.84
1:A:290:LEU:CD1	1:A:291:VAL:H	1.90	0.83
1:A:360:ILE:HD12	1:A:361:TYR:H	1.41	0.83
1:A:414:LYS:HZ2	1:A:419:LYS:HE2	1.42	0.83
1:A:245:ILE:HG23	1:A:245:ILE:O	1.78	0.83
1:A:393:TRP:CE2	1:A:421:PHE:HB2	2.15	0.82
1:A:211:ILE:C	1:A:211:ILE:HD12	2.00	0.81
1:A:84:LEU:CD2	1:A:88:LEU:HD12	2.11	0.81
1:A:182:GLY:O	1:A:183:GLU:HB2	1.79	0.80
1:A:334:LEU:CD1	1:A:360:ILE:HD13	2.08	0.80
1:A:380:VAL:O	1:A:383:VAL:HG12	1.83	0.79
1:A:41:LYS:HZ2	1:A:163:LEU:HD13	1.46	0.79
1:A:28:ILE:HD11	1:A:284:HIS:HB2	1.65	0.78
1:A:209:LYS:C	1:A:210:ILE:HG22	2.04	0.77
1:A:232:LEU:O	1:A:236:TYR:HB2	1.84	0.77
1:A:335:ARG:O	1:A:348:LEU:HB2	1.84	0.77
1:A:202:VAL:HG22	1:A:207:PRO:CG	2.14	0.77
1:A:46:VAL:CG2	1:A:46:VAL:O	2.32	0.77
1:A:77:LEU:HD23	1:A:77:LEU:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:O	1:A:210:ILE:HG13	1.84	0.76
1:A:120:ASN:O	1:A:124:VAL:HG23	1.85	0.76
1:A:109:LEU:HD21	1:A:154:LEU:HD22	1.68	0.76
1:A:427:ASN:O	1:A:431:ILE:HG12	1.85	0.76
1:A:26:LYS:HB3	1:A:27:GLU:OE2	1.86	0.76
1:A:46:VAL:HG22	1:A:46:VAL:O	1.86	0.75
1:A:414:LYS:NZ	1:A:419:LYS:HE2	2.00	0.75
1:A:164:ALA:HB3	1:A:165:PRO:HD3	1.68	0.75
1:A:194:ALA:O	1:A:197:ALA:HB3	1.87	0.74
1:A:34:ARG:NH1	1:A:370:ASP:HB2	2.02	0.74
1:A:295:GLU:OE2	1:A:341:ASN:HB2	1.88	0.74
1:A:209:LYS:HZ3	1:A:270:SER:HB2	1.52	0.74
1:A:75:ILE:O	1:A:75:ILE:HG13	1.87	0.74
1:A:289:THR:HG22	1:A:290:LEU:O	1.88	0.74
1:A:348:LEU:CD1	1:A:388:THR:HG21	2.18	0.74
1:A:158:VAL:O	1:A:158:VAL:CG2	2.36	0.74
1:A:43:PHE:CE2	1:A:72:LEU:HB3	2.21	0.73
1:A:292:ARG:HG2	1:A:292:ARG:NH1	1.97	0.73
1:A:267:SER:O	1:A:268:SER:CB	2.36	0.73
1:A:190:LEU:N	1:A:190:LEU:HD22	1.98	0.73
1:A:441:ARG:NH1	1:A:441:ARG:HG3	1.97	0.73
1:A:221:ASP:HA	1:A:244:TRP:CZ3	2.24	0.73
1:A:231:ASN:HD21	1:A:294:GLY:HA3	1.54	0.72
1:A:163:LEU:O	1:A:167:GLU:HG2	1.87	0.72
1:A:120:ASN:C	1:A:120:ASN:HD22	1.92	0.72
1:A:43:PHE:CG	1:A:44:ALA:N	2.57	0.72
1:A:41:LYS:HA	1:A:170:LEU:HD22	1.69	0.71
1:A:183:GLU:O	1:A:184:THR:O	2.08	0.71
1:A:149:ARG:HG3	1:A:150:ASP:OD1	1.89	0.71
1:A:219:LEU:CD2	1:A:289:THR:HG21	2.21	0.71
1:A:237:ASP:O	1:A:241:GLN:HG3	1.90	0.71
1:A:404:PHE:O	1:A:407:ALA:HB3	1.90	0.71
1:A:24:SER:HA	1:A:27:GLU:OE1	1.90	0.71
1:A:47:LYS:O	1:A:47:LYS:CG	2.39	0.71
1:A:158:VAL:O	1:A:158:VAL:HG23	1.90	0.71
1:A:209:LYS:NZ	1:A:270:SER:HB2	2.06	0.70
1:A:409:SER:HB2	1:A:421:PHE:HD2	1.56	0.70
1:A:290:LEU:CD1	1:A:291:VAL:N	2.55	0.70
1:A:106:PRO:C	1:A:108:ALA:H	1.95	0.70
1:A:218:GLY:HA2	1:A:271:ILE:HG12	1.72	0.70
1:A:209:LYS:HE3	1:A:210:ILE:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HD22	1:A:328:PHE:HB3	1.74	0.70
1:A:219:LEU:HD23	1:A:289:THR:HG21	1.72	0.70
1:A:203:GLN:NE2	1:A:262:ARG:HD3	2.07	0.69
1:A:344:ALA:HB2	1:A:376:LEU:HD13	1.74	0.69
1:A:209:LYS:HG3	1:A:281:LEU:HD22	1.74	0.69
1:A:109:LEU:CD1	1:A:154:LEU:HD13	2.22	0.69
1:A:247:GLY:O	1:A:250:ARG:HG3	1.93	0.69
1:A:124:VAL:HG11	1:A:136:SER:N	1.98	0.69
1:A:242:GLN:O	1:A:242:GLN:HG3	1.90	0.69
1:A:137:ILE:HD11	1:A:165:PRO:HB2	1.74	0.69
1:A:357:SER:HB2	1:A:358:ALA:CA	2.09	0.69
1:A:410:ASP:HB2	1:A:423:TYR:HA	1.74	0.69
1:A:76:VAL:CG1	1:A:77:LEU:N	2.56	0.69
1:A:49:GLY:O	1:A:52:VAL:HG12	1.93	0.68
1:A:337:TYR:HB2	1:A:346:VAL:CG2	2.16	0.68
1:A:209:LYS:O	1:A:210:ILE:CG2	2.37	0.68
1:A:392:PHE:CB	1:A:438:CYS:SG	2.81	0.68
1:A:210:ILE:O	1:A:210:ILE:CG1	2.41	0.68
1:A:269:VAL:O	1:A:270:SER:HB2	1.94	0.68
1:A:141:VAL:HG12	1:A:162:ASN:O	1.93	0.68
1:A:76:VAL:HG13	1:A:77:LEU:N	2.08	0.68
1:A:362:LEU:HB3	1:A:393:TRP:HB3	1.76	0.68
1:A:256:ILE:HG23	1:A:269:VAL:CG2	2.22	0.68
1:A:201:LEU:O	1:A:204:GLU:HG2	1.93	0.68
1:A:347:ILE:HD12	1:A:364:LYS:HG3	1.76	0.68
1:A:203:GLN:HE21	1:A:262:ARG:HD3	1.59	0.67
1:A:109:LEU:HD23	1:A:189:ILE:O	1.94	0.67
1:A:45:VAL:HG12	1:A:45:VAL:O	1.94	0.67
1:A:75:ILE:HD11	1:A:205:LEU:HD13	1.76	0.67
1:A:296:ARG:HG3	1:A:340:GLU:CB	2.24	0.67
1:A:393:TRP:NE1	1:A:421:PHE:HB2	2.10	0.67
1:A:237:ASP:C	1:A:239:LEU:H	1.94	0.67
1:A:41:LYS:NZ	1:A:163:LEU:HD13	2.09	0.67
1:A:77:LEU:CD2	1:A:77:LEU:O	2.42	0.67
1:A:263:LEU:HB3	1:A:264:PRO:CD	2.25	0.67
1:A:78:HIS:NE2	1:A:179:THR:HG22	2.09	0.67
1:A:267:SER:O	1:A:268:SER:HB3	1.94	0.67
1:A:360:ILE:HD12	1:A:361:TYR:N	2.11	0.66
1:A:442:GLN:HA	1:A:445:LEU:CD1	2.26	0.66
1:A:44:ALA:O	1:A:45:VAL:HG23	1.94	0.66
1:A:109:LEU:CD2	1:A:154:LEU:HD22	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD11	1:A:165:PRO:CB	2.25	0.66
1:A:188:GLN:NE2	1:A:189:ILE:H	1.92	0.66
1:A:228:ASP:O	1:A:229:SER:HB2	1.95	0.66
1:A:254:GLU:O	1:A:257:LYS:HB3	1.95	0.66
1:A:316:GLU:HB2	1:A:322:THR:HG22	1.78	0.65
1:A:347:ILE:HD12	1:A:364:LYS:HB2	1.77	0.65
1:A:361:TYR:CZ	1:A:445:LEU:HD13	2.31	0.65
1:A:408:GLU:HA	1:A:408:GLU:OE2	1.96	0.65
1:A:12:ARG:HA	1:A:15:ILE:CG2	2.24	0.65
1:A:272:THR:OG1	1:A:273:ARG:N	2.29	0.65
1:A:214:THR:HG22	1:A:216:THR:HG23	1.79	0.65
1:A:341:ASN:HD22	1:A:343:ARG:NE	1.92	0.65
1:A:236:TYR:CZ	1:A:240:MSE:HG2	2.32	0.65
1:A:211:ILE:CD1	1:A:213:LEU:N	2.60	0.65
1:A:341:ASN:ND2	1:A:343:ARG:HE	1.94	0.65
1:A:41:LYS:HZ3	1:A:167:GLU:HB3	1.60	0.64
1:A:290:LEU:C	1:A:291:VAL:HG12	2.17	0.64
1:A:190:LEU:H	1:A:190:LEU:CD2	2.07	0.64
1:A:203:GLN:NE2	1:A:262:ARG:HH11	1.96	0.64
1:A:150:ASP:OD1	1:A:150:ASP:N	2.30	0.64
1:A:303:TRP:CE3	1:A:333:LEU:HB3	2.32	0.64
1:A:211:ILE:HD11	1:A:213:LEU:N	2.13	0.64
1:A:135:THR:O	1:A:135:THR:OG1	2.14	0.64
1:A:290:LEU:HD13	1:A:291:VAL:N	2.07	0.64
1:A:12:ARG:HE	1:A:36:SER:CB	2.11	0.63
1:A:344:ALA:CB	1:A:376:LEU:HD13	2.27	0.63
1:A:103:VAL:HG23	1:A:152:TYR:O	1.99	0.63
1:A:16:VAL:HA	1:A:19:LEU:HD12	1.79	0.63
1:A:426:GLU:HB2	1:A:431:ILE:HG23	1.80	0.63
1:A:156:GLY:O	1:A:192:VAL:HG12	1.99	0.63
1:A:42:ARG:HH21	1:A:206:GLN:HB3	1.61	0.63
1:A:209:LYS:C	1:A:210:ILE:CG2	2.68	0.63
1:A:188:GLN:NE2	1:A:189:ILE:N	2.38	0.62
1:A:133:ARG:O	1:A:174:SER:CB	2.46	0.62
1:A:170:LEU:HD11	1:A:176:PRO:HG2	1.81	0.62
1:A:210:ILE:CD1	1:A:212:PHE:HE1	1.97	0.62
1:A:12:ARG:HE	1:A:36:SER:HB2	1.64	0.62
1:A:177:VAL:CG2	1:A:177:VAL:O	2.48	0.62
1:A:196:PHE:N	1:A:196:PHE:CD1	2.65	0.62
1:A:290:LEU:O	1:A:291:VAL:CG1	2.42	0.62
1:A:39:ASP:OD1	1:A:42:ARG:HD3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:VAL:HG23	1:A:49:GLY:N	2.15	0.61
1:A:202:VAL:HG12	1:A:203:GLN:N	2.14	0.61
1:A:84:LEU:C	1:A:84:LEU:HD23	2.21	0.61
1:A:240:MSE:HE1	1:A:250:ARG:HB3	1.82	0.61
1:A:291:VAL:O	1:A:291:VAL:HG22	2.01	0.61
1:A:327:TYR:O	1:A:331:THR:HG23	2.01	0.61
1:A:211:ILE:C	1:A:211:ILE:CD1	2.65	0.61
1:A:213:LEU:HD11	1:A:277:LEU:CD1	2.30	0.61
1:A:95:LYS:O	1:A:96:GLN:CB	2.49	0.61
1:A:357:SER:CB	1:A:358:ALA:CA	2.72	0.60
1:A:164:ALA:HA	1:A:167:GLU:HG3	1.83	0.60
1:A:210:ILE:HD12	1:A:210:ILE:C	2.22	0.60
1:A:77:LEU:HD12	1:A:201:LEU:CD2	2.29	0.60
1:A:182:GLY:O	1:A:183:GLU:CB	2.48	0.60
1:A:75:ILE:HD11	1:A:205:LEU:CD1	2.32	0.60
1:A:430:GLN:O	1:A:434:CYS:SG	2.60	0.60
1:A:41:LYS:CG	1:A:170:LEU:HD13	2.32	0.60
1:A:311:LEU:HA	1:A:314:LEU:HB3	1.83	0.60
1:A:226:LEU:HD11	1:A:287:SER:O	2.02	0.60
1:A:334:LEU:CD2	1:A:335:ARG:HB2	2.32	0.59
1:A:75:ILE:CG1	1:A:75:ILE:O	2.50	0.59
1:A:16:VAL:HG13	1:A:29:SER:HB2	1.83	0.59
1:A:337:TYR:OH	1:A:387:GLU:HG2	2.02	0.59
1:A:95:LYS:O	1:A:96:GLN:HB2	2.00	0.59
1:A:231:ASN:ND2	1:A:231:ASN:O	2.26	0.59
1:A:408:GLU:O	1:A:409:SER:C	2.41	0.59
1:A:109:LEU:CD1	1:A:109:LEU:H	2.14	0.59
1:A:109:LEU:N	1:A:109:LEU:HD12	2.13	0.59
1:A:109:LEU:HD13	1:A:154:LEU:HD13	1.84	0.59
1:A:84:LEU:O	1:A:84:LEU:HD23	2.01	0.59
1:A:348:LEU:HD11	1:A:388:THR:HG21	1.85	0.58
1:A:343:ARG:HG2	1:A:368:LEU:HD12	1.85	0.58
1:A:371:ALA:C	1:A:373:GLY:H	2.06	0.58
1:A:132:ALA:O	1:A:133:ARG:HG3	2.03	0.58
1:A:371:ALA:C	1:A:373:GLY:N	2.56	0.58
1:A:296:ARG:HG3	1:A:340:GLU:HB3	1.86	0.58
1:A:219:LEU:HB2	1:A:289:THR:OG1	2.03	0.58
1:A:347:ILE:HD12	1:A:364:LYS:CB	2.33	0.58
1:A:285:LYS:HG3	1:A:286:GLY:N	2.19	0.58
1:A:361:TYR:OH	1:A:445:LEU:HD13	2.04	0.58
1:A:154:LEU:HD23	1:A:190:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:O	1:A:153:GLY:HA2	2.03	0.58
1:A:177:VAL:HG22	1:A:177:VAL:O	2.04	0.58
1:A:109:LEU:HD11	1:A:154:LEU:HD13	1.86	0.57
1:A:234:THR:OG1	1:A:235:GLU:N	2.37	0.57
1:A:41:LYS:HG3	1:A:170:LEU:HD13	1.85	0.57
1:A:211:ILE:HG13	1:A:211:ILE:O	2.04	0.57
1:A:391:LEU:O	1:A:422:TRP:HA	2.03	0.57
1:A:99:ASN:CG	1:A:100:GLY:H	2.07	0.57
1:A:208:TYR:CD2	1:A:209:LYS:N	2.73	0.57
1:A:38:LEU:HD12	1:A:42:ARG:NH1	2.20	0.57
1:A:175:ILE:O	1:A:177:VAL:HG12	2.04	0.57
1:A:124:VAL:HG13	1:A:134:ALA:HB1	1.85	0.56
1:A:110:ALA:O	1:A:114:LYS:HG3	2.05	0.56
1:A:124:VAL:HG21	1:A:136:SER:HB2	1.87	0.56
1:A:441:ARG:CG	1:A:441:ARG:NH1	2.68	0.56
1:A:144:ALA:HB3	1:A:182:GLY:HA3	1.87	0.56
1:A:271:ILE:O	1:A:271:ILE:HG12	2.05	0.56
1:A:43:PHE:CD2	1:A:72:LEU:HB3	2.40	0.56
1:A:442:GLN:HG2	1:A:445:LEU:HD11	1.87	0.56
1:A:269:VAL:CG1	1:A:270:SER:N	2.48	0.56
1:A:106:PRO:O	1:A:108:ALA:N	2.38	0.56
1:A:190:LEU:N	1:A:190:LEU:CD2	2.67	0.56
1:A:12:ARG:NE	1:A:36:SER:CB	2.69	0.56
1:A:271:ILE:O	1:A:271:ILE:CG1	2.53	0.56
1:A:308:LEU:HB2	1:A:309:PRO:HD3	1.88	0.56
1:A:418:TRP:HZ2	1:A:446:LEU:HD12	1.70	0.56
1:A:10:GLN:HG3	1:A:11:THR:H	1.70	0.56
1:A:259:LEU:O	1:A:261:ASP:N	2.39	0.55
1:A:378:ARG:O	1:A:382:ASN:HB2	2.06	0.55
1:A:109:LEU:HD21	1:A:154:LEU:HB3	1.87	0.55
1:A:145:GLU:OE1	1:A:159:LYS:HD3	2.05	0.55
1:A:15:ILE:O	1:A:19:LEU:HG	2.06	0.55
1:A:339:SER:O	1:A:341:ASN:N	2.40	0.55
1:A:409:SER:CB	1:A:421:PHE:HD2	2.19	0.55
1:A:143:GLU:HG2	1:A:159:LYS:HZ3	1.71	0.55
1:A:305:GLU:O	1:A:306:LEU:HD23	2.06	0.55
1:A:176:PRO:O	1:A:178:ILE:HG13	2.06	0.55
1:A:178:ILE:CG2	1:A:179:THR:N	2.55	0.55
1:A:305:GLU:C	1:A:306:LEU:HD23	2.27	0.55
1:A:240:MSE:C	1:A:241:GLN:HG2	2.26	0.55
1:A:390:GLN:OE1	1:A:424:GLY:HA3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ILE:O	1:A:177:VAL:N	2.39	0.54
1:A:230:ILE:HB	1:A:291:VAL:HB	1.90	0.54
1:A:341:ASN:O	1:A:342:TYR:HB2	2.07	0.54
1:A:399:ASN:HB3	1:A:402:ASN:OD1	2.07	0.54
1:A:163:LEU:HG	1:A:204:GLU:CD	2.28	0.54
1:A:408:GLU:O	1:A:409:SER:O	2.25	0.54
1:A:323:LEU:HD13	1:A:327:TYR:CD2	2.43	0.54
1:A:347:ILE:HD12	1:A:364:LYS:CG	2.37	0.54
1:A:199:ASN:HB2	1:A:255:GLN:HE22	1.72	0.54
1:A:81:GLY:H	1:A:82:PRO:CD	2.21	0.54
1:A:113:ARG:HD3	1:A:189:ILE:HD11	1.90	0.54
1:A:296:ARG:HG3	1:A:340:GLU:HB2	1.89	0.54
1:A:105:SER:O	1:A:109:LEU:HD12	2.08	0.54
1:A:105:SER:HB2	1:A:106:PRO:HD2	1.89	0.54
1:A:290:LEU:HD12	1:A:292:ARG:HD2	1.90	0.54
1:A:75:ILE:CD1	1:A:205:LEU:HD11	2.37	0.54
1:A:144:ALA:CB	1:A:182:GLY:HA3	2.38	0.54
1:A:405:TYR:O	1:A:407:ALA:N	2.40	0.54
1:A:127:LEU:HB3	1:A:132:ALA:HB3	1.89	0.54
1:A:106:PRO:C	1:A:108:ALA:N	2.61	0.54
1:A:242:GLN:O	1:A:242:GLN:CG	2.56	0.54
1:A:32:LEU:O	1:A:36:SER:HB3	2.07	0.53
1:A:166:ILE:HD13	1:A:178:ILE:CD1	2.37	0.53
1:A:239:LEU:HA	1:A:242:GLN:HG2	1.90	0.53
1:A:323:LEU:HD11	1:A:364:LYS:HE2	1.89	0.53
1:A:303:TRP:HE3	1:A:333:LEU:HB3	1.72	0.53
1:A:211:ILE:HD11	1:A:213:LEU:H	1.73	0.53
1:A:229:SER:O	1:A:230:ILE:HG12	2.09	0.53
1:A:227:ILE:O	1:A:229:SER:N	2.37	0.53
1:A:12:ARG:NE	1:A:36:SER:HB2	2.23	0.53
1:A:42:ARG:HE	1:A:206:GLN:HB2	1.73	0.53
1:A:111:ILE:O	1:A:115:VAL:CG2	2.52	0.53
1:A:222:ALA:HB2	1:A:244:TRP:CD1	2.43	0.53
1:A:50:GLY:HA3	1:A:80:ALA:HA	1.90	0.53
1:A:67:LEU:O	1:A:70:VAL:HG22	2.09	0.53
1:A:84:LEU:C	1:A:84:LEU:CD2	2.77	0.53
1:A:440:THR:C	1:A:443:PRO:HD2	2.30	0.52
1:A:12:ARG:HH21	1:A:36:SER:HB2	1.74	0.52
1:A:300:ALA:HB3	1:A:336:ALA:HB3	1.89	0.52
1:A:263:LEU:HB3	1:A:264:PRO:HD2	1.92	0.52
1:A:414:LYS:O	1:A:415:GLN:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:CD1	1:A:205:LEU:CD1	2.88	0.52
1:A:334:LEU:HD22	1:A:335:ARG:HB2	1.92	0.52
1:A:387:GLU:HG3	1:A:388:THR:CG2	2.40	0.52
1:A:380:VAL:HG12	1:A:381:TRP:N	2.25	0.52
1:A:393:TRP:NE1	1:A:421:PHE:CD1	2.77	0.52
1:A:143:GLU:HG2	1:A:159:LYS:NZ	2.24	0.52
1:A:428:PHE:HA	1:A:431:ILE:HD11	1.92	0.52
1:A:211:ILE:HD12	1:A:212:PHE:CA	2.40	0.52
1:A:381:TRP:NE1	1:A:408:GLU:HG3	2.25	0.52
1:A:442:GLN:N	1:A:443:PRO:CD	2.73	0.52
1:A:371:ALA:O	1:A:373:GLY:N	2.43	0.51
1:A:109:LEU:O	1:A:112:VAL:N	2.43	0.51
1:A:188:GLN:HE21	1:A:188:GLN:C	2.13	0.51
1:A:314:LEU:HD13	1:A:342:TYR:O	2.11	0.51
1:A:384:MSE:C	1:A:386:GLU:H	2.14	0.51
1:A:264:PRO:HD2	1:A:267:SER:OG	2.11	0.51
1:A:124:VAL:CG1	1:A:136:SER:H	2.04	0.51
1:A:161:VAL:HB	1:A:204:GLU:CD	2.31	0.51
1:A:260:LEU:HD21	1:A:269:VAL:H	1.75	0.51
1:A:109:LEU:HA	1:A:112:VAL:HG22	1.93	0.50
1:A:408:GLU:CA	1:A:408:GLU:OE2	2.58	0.50
1:A:148:ASN:HB3	1:A:152:TYR:HD2	1.76	0.50
1:A:219:LEU:HD22	1:A:289:THR:HG21	1.94	0.50
1:A:242:GLN:NE2	1:A:244:TRP:CZ2	2.79	0.50
1:A:213:LEU:CD2	1:A:274:PRO:HG3	2.30	0.50
1:A:120:ASN:C	1:A:120:ASN:ND2	2.62	0.50
1:A:27:GLU:CD	1:A:27:GLU:H	2.14	0.50
1:A:143:GLU:O	1:A:143:GLU:CG	2.59	0.50
1:A:307:ASP:CG	1:A:310:ARG:HG3	2.32	0.50
1:A:127:LEU:HD22	1:A:175:ILE:CD1	2.38	0.50
1:A:137:ILE:CG1	1:A:137:ILE:O	2.45	0.50
1:A:39:ASP:OD1	1:A:42:ARG:HB2	2.11	0.50
1:A:260:LEU:C	1:A:262:ARG:H	2.15	0.49
1:A:401:VAL:HG22	1:A:401:VAL:O	2.11	0.49
1:A:236:TYR:OH	1:A:240:MSE:HG2	2.12	0.49
1:A:243:PRO:C	1:A:245:ILE:H	2.15	0.49
1:A:78:HIS:CE1	1:A:179:THR:HG22	2.47	0.49
1:A:112:VAL:O	1:A:115:VAL:N	2.45	0.49
1:A:245:ILE:CG2	1:A:245:ILE:O	2.50	0.49
1:A:339:SER:O	1:A:340:GLU:C	2.50	0.49
1:A:208:TYR:CG	1:A:209:LYS:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:C	1:A:77:LEU:HD23	2.33	0.49
1:A:288:GLY:O	1:A:289:THR:C	2.52	0.49
1:A:381:TRP:CE2	1:A:408:GLU:HG3	2.48	0.49
1:A:237:ASP:O	1:A:239:LEU:N	2.39	0.49
1:A:442:GLN:HA	1:A:445:LEU:HD11	1.94	0.48
1:A:315:ILE:HD12	1:A:316:GLU:N	2.28	0.48
1:A:292:ARG:NH1	1:A:292:ARG:CG	2.57	0.48
1:A:80:ALA:HB1	1:A:83:GLN:OE1	2.12	0.48
1:A:41:LYS:CG	1:A:205:LEU:HD11	2.44	0.48
1:A:289:THR:C	1:A:290:LEU:O	2.48	0.48
1:A:237:ASP:C	1:A:239:LEU:N	2.65	0.48
1:A:147:LEU:HD22	1:A:148:ASN:H	1.79	0.48
1:A:10:GLN:O	1:A:13:GLN:HB3	2.14	0.48
1:A:334:LEU:HD23	1:A:335:ARG:HB2	1.94	0.48
1:A:409:SER:HB2	1:A:421:PHE:CD2	2.43	0.48
1:A:332:LYS:O	1:A:349:THR:HG22	2.13	0.48
1:A:93:ILE:HG22	1:A:93:ILE:O	2.13	0.48
1:A:137:ILE:HD13	1:A:165:PRO:O	2.14	0.48
1:A:12:ARG:CA	1:A:15:ILE:HG22	2.35	0.48
1:A:216:THR:OG1	1:A:217:GLY:N	2.45	0.48
1:A:77:LEU:CD1	1:A:201:LEU:HD23	2.36	0.48
1:A:37:GLN:O	1:A:38:LEU:HB2	2.12	0.48
1:A:380:VAL:CG1	1:A:381:TRP:N	2.77	0.48
1:A:143:GLU:O	1:A:145:GLU:N	2.46	0.48
1:A:290:LEU:C	1:A:291:VAL:CG1	2.83	0.47
1:A:75:ILE:HG22	1:A:170:LEU:HD21	1.95	0.47
1:A:239:LEU:C	1:A:241:GLN:H	2.16	0.47
1:A:438:CYS:O	1:A:442:GLN:OE1	2.32	0.47
1:A:442:GLN:HA	1:A:445:LEU:HG	1.96	0.47
1:A:211:ILE:HD12	1:A:213:LEU:N	2.29	0.47
1:A:12:ARG:NH2	1:A:36:SER:HB2	2.28	0.47
1:A:193:ASN:HD22	1:A:194:ALA:N	2.12	0.47
1:A:41:LYS:NZ	1:A:167:GLU:HB3	2.28	0.47
1:A:260:LEU:C	1:A:262:ARG:N	2.68	0.47
1:A:27:GLU:CD	1:A:27:GLU:N	2.67	0.47
1:A:94:GLU:O	1:A:94:GLU:HG3	2.14	0.47
1:A:212:PHE:HD1	1:A:212:PHE:N	2.11	0.47
1:A:266:GLU:O	1:A:267:SER:O	2.32	0.47
1:A:18:LEU:O	1:A:22:MSE:SE	2.82	0.47
1:A:72:LEU:O	1:A:74:PRO:HD3	2.14	0.47
1:A:393:TRP:CE2	1:A:421:PHE:CB	2.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:THR:HB	1:A:185:PRO:CD	2.45	0.47
1:A:99:ASN:CG	1:A:100:GLY:N	2.68	0.47
1:A:81:GLY:H	1:A:82:PRO:HD3	1.80	0.47
1:A:193:ASN:OD1	1:A:196:PHE:CZ	2.68	0.47
1:A:101:LEU:HD11	1:A:196:PHE:HE2	1.80	0.47
1:A:127:LEU:C	1:A:132:ALA:HB3	2.36	0.46
1:A:212:PHE:CD1	1:A:212:PHE:N	2.82	0.46
1:A:53:LEU:HD12	1:A:57:LEU:HD13	1.97	0.46
1:A:360:ILE:CG2	1:A:390:GLN:O	2.64	0.46
1:A:227:ILE:O	1:A:227:ILE:HG12	2.15	0.46
1:A:380:VAL:HG12	1:A:381:TRP:H	1.81	0.46
1:A:262:ARG:C	1:A:263:LEU:HD23	2.36	0.46
1:A:291:VAL:O	1:A:291:VAL:CG2	2.62	0.46
1:A:99:ASN:HB2	1:A:152:TYR:OH	2.15	0.46
1:A:426:GLU:O	1:A:431:ILE:HG23	2.16	0.46
1:A:166:ILE:HD13	1:A:178:ILE:HD11	1.97	0.46
1:A:109:LEU:HD11	1:A:154:LEU:CB	2.44	0.46
1:A:50:GLY:CA	1:A:80:ALA:HA	2.46	0.46
1:A:391:LEU:HG	1:A:393:TRP:CE3	2.51	0.46
1:A:367:VAL:HG21	1:A:372:GLN:OE1	2.15	0.46
1:A:290:LEU:HD12	1:A:291:VAL:N	2.28	0.45
1:A:16:VAL:O	1:A:19:LEU:HB2	2.16	0.45
1:A:135:THR:CG2	1:A:174:SER:CB	2.94	0.45
1:A:210:ILE:O	1:A:210:ILE:CD1	2.63	0.45
1:A:394:ARG:NH2	1:A:446:LEU:HG	2.32	0.45
1:A:388:THR:HA	1:A:389:PRO:HD3	1.63	0.45
1:A:211:ILE:HD11	1:A:213:LEU:CD1	2.26	0.45
1:A:232:LEU:O	1:A:236:TYR:CB	2.58	0.45
1:A:39:ASP:CG	1:A:42:ARG:HD3	2.36	0.45
1:A:428:PHE:O	1:A:431:ILE:HG13	2.16	0.45
1:A:209:LYS:HE2	1:A:281:LEU:CD2	2.47	0.45
1:A:323:LEU:HD22	1:A:327:TYR:CG	2.52	0.45
1:A:394:ARG:HD2	1:A:418:TRP:CZ3	2.52	0.45
1:A:362:LEU:HD23	1:A:393:TRP:CB	2.47	0.45
1:A:157:GLU:O	1:A:159:LYS:N	2.50	0.45
1:A:81:GLY:N	1:A:82:PRO:CD	2.78	0.45
1:A:438:CYS:O	1:A:442:GLN:HB2	2.16	0.45
1:A:259:LEU:O	1:A:262:ARG:N	2.44	0.45
1:A:401:VAL:HG22	1:A:404:PHE:HB3	1.99	0.45
1:A:138:THR:O	1:A:138:THR:HG22	2.17	0.45
1:A:166:ILE:HG23	1:A:176:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:NH1	1:A:370:ASP:O	2.50	0.44
1:A:127:LEU:HD13	1:A:175:ILE:HG13	1.99	0.44
1:A:327:TYR:CE2	1:A:331:THR:CG2	3.00	0.44
1:A:164:ALA:HB3	1:A:165:PRO:CD	2.42	0.44
1:A:261:ASP:OD1	1:A:293:ARG:HD2	2.17	0.44
1:A:225:LYS:HD2	1:A:225:LYS:HA	1.75	0.44
1:A:231:ASN:C	1:A:231:ASN:HD22	2.14	0.44
1:A:206:GLN:O	1:A:207:PRO:O	2.34	0.44
1:A:38:LEU:O	1:A:39:ASP:O	2.35	0.44
1:A:369:ASP:C	1:A:371:ALA:H	2.20	0.44
1:A:143:GLU:OE1	1:A:159:LYS:HE2	2.16	0.44
1:A:209:LYS:HD2	1:A:209:LYS:HA	1.72	0.44
1:A:211:ILE:HD12	1:A:212:PHE:C	2.37	0.44
1:A:310:ARG:CZ	1:A:342:TYR:HB2	2.48	0.44
1:A:42:ARG:HG2	1:A:205:LEU:O	2.17	0.44
1:A:311:LEU:HD23	1:A:314:LEU:HD23	2.00	0.44
1:A:343:ARG:HA	1:A:368:LEU:HD12	1.99	0.44
1:A:360:ILE:HG23	1:A:390:GLN:O	2.16	0.44
1:A:109:LEU:HD11	1:A:154:LEU:HB2	1.99	0.44
1:A:154:LEU:O	1:A:190:LEU:HB2	2.17	0.44
1:A:154:LEU:C	1:A:190:LEU:HB2	2.39	0.43
1:A:385:ARG:HD2	1:A:385:ARG:O	2.18	0.43
1:A:210:ILE:O	1:A:210:ILE:HD12	2.18	0.43
1:A:242:GLN:NE2	1:A:244:TRP:CE2	2.86	0.43
1:A:387:GLU:HG3	1:A:388:THR:HG23	2.00	0.43
1:A:209:LYS:HZ3	1:A:270:SER:CB	2.27	0.43
1:A:41:LYS:HZ3	1:A:167:GLU:CB	2.28	0.43
1:A:41:LYS:O	1:A:205:LEU:HD21	2.18	0.43
1:A:16:VAL:HA	1:A:19:LEU:HB2	2.00	0.43
1:A:381:TRP:CZ2	1:A:408:GLU:HG3	2.54	0.43
1:A:405:TYR:O	1:A:406:TYR:C	2.56	0.43
1:A:78:HIS:CD2	1:A:178:ILE:O	2.71	0.43
1:A:242:GLN:HA	1:A:243:PRO:HD3	1.55	0.43
1:A:219:LEU:O	1:A:220:LEU:HD23	2.19	0.43
1:A:310:ARG:HD3	1:A:342:TYR:CD1	2.54	0.43
1:A:35:PHE:CE1	1:A:208:TYR:HB2	2.54	0.43
1:A:41:LYS:HG2	1:A:205:LEU:HD11	1.99	0.43
1:A:258:ASP:O	1:A:259:LEU:O	2.36	0.43
1:A:315:ILE:HD12	1:A:315:ILE:C	2.39	0.43
1:A:265:LEU:HD11	1:A:293:ARG:NH2	2.34	0.42
1:A:414:LYS:NZ	1:A:419:LYS:CE	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASN:OD1	1:A:247:GLY:N	2.51	0.42
1:A:387:GLU:HG3	1:A:388:THR:HG22	2.01	0.42
1:A:230:ILE:HG22	1:A:231:ASN:N	2.34	0.42
1:A:140:GLY:HA2	1:A:183:GLU:OE1	2.19	0.42
1:A:109:LEU:O	1:A:112:VAL:HG22	2.19	0.42
1:A:411:GLY:HA3	1:A:422:TRP:CZ2	2.53	0.42
1:A:283:THR:OG1	1:A:286:GLY:N	2.51	0.42
1:A:48:VAL:CG2	1:A:78:HIS:HA	2.48	0.42
1:A:227:ILE:O	1:A:227:ILE:CG1	2.67	0.42
1:A:232:LEU:HG	1:A:232:LEU:H	1.48	0.42
1:A:280:GLU:HA	1:A:286:GLY:HA3	2.01	0.42
1:A:60:LEU:O	1:A:64:LEU:HD12	2.19	0.42
1:A:442:GLN:HA	1:A:445:LEU:CG	2.49	0.42
1:A:135:THR:CG2	1:A:174:SER:HB3	2.50	0.42
1:A:267:SER:O	1:A:268:SER:OG	2.37	0.42
1:A:44:ALA:O	1:A:45:VAL:CG2	2.65	0.42
1:A:26:LYS:CB	1:A:27:GLU:OE2	2.62	0.42
1:A:252:LYS:HD3	1:A:252:LYS:O	2.20	0.42
1:A:200:GLU:HG3	1:A:200:GLU:O	2.19	0.42
1:A:368:LEU:O	1:A:371:ALA:HB3	2.19	0.42
1:A:263:LEU:N	1:A:263:LEU:HD23	2.35	0.42
1:A:367:VAL:HG11	1:A:377:GLY:CA	2.49	0.42
1:A:95:LYS:O	1:A:96:GLN:CG	2.68	0.42
1:A:256:ILE:O	1:A:260:LEU:CD1	2.55	0.42
1:A:341:ASN:ND2	1:A:343:ARG:NE	2.61	0.42
1:A:176:PRO:O	1:A:178:ILE:CG1	2.68	0.41
1:A:163:LEU:C	1:A:167:GLU:HG2	2.40	0.41
1:A:167:GLU:O	1:A:171:GLN:HB2	2.21	0.41
1:A:239:LEU:CA	1:A:242:GLN:HG2	2.49	0.41
1:A:371:ALA:O	1:A:374:GLU:N	2.54	0.41
1:A:408:GLU:C	1:A:409:SER:O	2.57	0.41
1:A:99:ASN:C	1:A:101:LEU:H	2.24	0.41
1:A:210:ILE:CD1	1:A:212:PHE:CE1	2.85	0.41
1:A:288:GLY:O	1:A:290:LEU:N	2.54	0.41
1:A:402:ASN:O	1:A:405:TYR:HB2	2.20	0.41
1:A:108:ALA:O	1:A:109:LEU:C	2.59	0.41
1:A:147:LEU:HD13	1:A:156:GLY:HA2	2.02	0.41
1:A:446:LEU:O	1:A:447:GLY:C	2.58	0.41
1:A:161:VAL:HB	1:A:204:GLU:OE1	2.21	0.41
1:A:84:LEU:O	1:A:88:LEU:HB2	2.21	0.41
1:A:419:LYS:HD3	1:A:421:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:CYS:HB2	1:A:419:LYS:NZ	2.36	0.41
1:A:99:ASN:C	1:A:101:LEU:N	2.74	0.41
1:A:163:LEU:HG	1:A:204:GLU:OE1	2.21	0.40
1:A:244:TRP:O	1:A:244:TRP:HE3	2.04	0.40
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.86	0.40
1:A:135:THR:CG2	1:A:174:SER:HB2	2.51	0.40
1:A:209:LYS:NZ	1:A:269:VAL:O	2.54	0.40
1:A:369:ASP:O	1:A:371:ALA:N	2.52	0.40
1:A:196:PHE:HD1	1:A:196:PHE:N	2.14	0.40
1:A:142:PHE:CD1	1:A:161:VAL:CG1	3.04	0.40
1:A:225:LYS:O	1:A:227:ILE:HG22	2.22	0.40
1:A:263:LEU:HD12	1:A:267:SER:CB	2.51	0.40
1:A:35:PHE:O	1:A:35:PHE:CG	2.75	0.40
1:A:27:GLU:HB3	1:A:372:GLN:O	2.21	0.40
1:A:24:SER:CA	1:A:27:GLU:OE1	2.63	0.40
1:A:279:LYS:O	1:A:283:THR:HG23	2.22	0.40
1:A:279:LYS:HB3	1:A:286:GLY:HA2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	436/467 (93%)	281 (64%)	90 (21%)	65 (15%)	0 0

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	39	ASP
1	A	46	VAL
1	A	76	VAL

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Mol	Chain	Res	Type
1	A	96	GLN
1	A	98	VAL
1	A	133	ARG
1	A	136	SER
1	A	138	THR
1	A	144	ALA
1	A	145	GLU
1	A	158	VAL
1	A	183	GLU
1	A	184	THR
1	A	210	ILE
1	A	228	ASP
1	A	232	LEU
1	A	246	ASN
1	A	259	LEU
1	A	267	SER
1	A	268	SER
1	A	269	VAL
1	A	270	SER
1	A	271	ILE
1	A	291	VAL
1	A	409	SER
1	A	37	GLN
1	A	45	VAL
1	A	93	ILE
1	A	107	HIS
1	A	132	ALA
1	A	143	GLU
1	A	176	PRO
1	A	260	LEU
1	A	285	LYS
1	A	289	THR
1	A	290	LEU
1	A	406	TYR
1	A	427	ASN
1	A	20	SER
1	A	78	HIS
1	A	110	ALA
1	A	185	PRO
1	A	264	PRO
1	A	303	TRP
1	A	357	SER

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Mol	Chain	Res	Type
1	A	370	ASP
1	A	385	ARG
1	A	396	ARG
1	A	80	ALA
1	A	177	VAL
1	A	321	ARG
1	A	382	ASN
1	A	401	VAL
1	A	65	SER
1	A	207	PRO
1	A	287	SER
1	A	340	GLU
1	A	405	TYR
1	A	432	GLN
1	A	48	VAL
1	A	372	GLN
1	A	79	GLY
1	A	320	GLY
1	A	263	LEU

### 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	366/384 (95%)	280 (76%)	86 (24%)	<b>1</b> <b>2</b>

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	31	TYR
1	A	38	LEU
1	A	39	ASP
1	A	46	VAL
1	A	47	LYS
1	A	53	LEU

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	75	ILE
1	A	83	GLN
1	A	88	LEU
1	A	107	HIS
1	A	111	ILE
1	A	115	VAL
1	A	120	ASN
1	A	124	VAL
1	A	128	GLN
1	A	135	THR
1	A	137	ILE
1	A	141	VAL
1	A	147	LEU
1	A	149	ARG
1	A	150	ASP
1	A	154	LEU
1	A	161	VAL
1	A	166	ILE
1	A	167	GLU
1	A	169	SER
1	A	171	GLN
1	A	175	ILE
1	A	177	VAL
1	A	180	SER
1	A	184	THR
1	A	188	GLN
1	A	189	ILE
1	A	190	LEU
1	A	193	ASN
1	A	196	PHE
1	A	201	LEU
1	A	202	VAL
1	A	205	LEU
1	A	210	ILE
1	A	211	ILE
1	A	213	LEU
1	A	219	LEU
1	A	227	ILE
1	A	231	ASN
1	A	234	THR
1	A	237	ASP

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Mol	Chain	Res	Type
1	A	239	LEU
1	A	241	GLN
1	A	252	LYS
1	A	253	ILE
1	A	258	ASP
1	A	259	LEU
1	A	266	GLU
1	A	271	ILE
1	A	272	THR
1	A	290	LEU
1	A	291	VAL
1	A	292	ARG
1	A	296	ARG
1	A	301	THR
1	A	305	GLU
1	A	306	LEU
1	A	321	ARG
1	A	327	TYR
1	A	340	GLU
1	A	351	GLU
1	A	365	PHE
1	A	367	VAL
1	A	370	ASP
1	A	376	LEU
1	A	380	VAL
1	A	382	ASN
1	A	384	MSE
1	A	385	ARG
1	A	388	THR
1	A	397	HIS
1	A	409	SER
1	A	410	ASP
1	A	415	GLN
1	A	429	GLU
1	A	431	ILE
1	A	434	CYS
1	A	438	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN

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Mol	Chain	Res	Type
1	A	193	ASN
1	A	203	GLN
1	A	206	GLN
1	A	231	ASN
1	A	255	GLN
1	A	341	ASN
1	A	382	ASN
1	A	415	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 carbohydrates 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	433/467 (92%)	1.37	99 (22%) <b>1</b> <b>1</b>	72, 162, 362, 557	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	PHE	16.7
1	A	355	GLY	11.5
1	A	328	PHE	10.8
1	A	354	LEU	10.3
1	A	24	SER	9.1
1	A	101	LEU	8.9
1	A	26	LYS	8.9
1	A	94	GLU	8.9
1	A	17	ARG	8.5
1	A	442	GLN	8.4
1	A	356	ALA	8.4
1	A	396	ARG	8.4
1	A	29	SER	8.3
1	A	97	THR	8.0
1	A	100	GLY	7.2
1	A	33	LYS	6.8
1	A	323	LEU	6.7
1	A	25	ALA	6.6
1	A	284	HIS	6.5
1	A	418	TRP	6.4
1	A	394	ARG	6.3
1	A	430	GLN	6.1
1	A	447	GLY	5.9
1	A	395	SER	5.9
1	A	357	SER	5.7
1	A	93	ILE	5.5
1	A	303	TRP	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	96	GLN	5.2
1	A	30	GLN	5.1
1	A	31	TYR	5.1
1	A	324	VAL	5.0
1	A	319	PHE	4.7
1	A	446	LEU	4.4
1	A	151	THR	4.2
1	A	368	LEU	4.2
1	A	327	TYR	4.2
1	A	443	PRO	4.2
1	A	21	SER	4.1
1	A	348	LEU	4.1
1	A	301	THR	4.0
1	A	325	PRO	4.0
1	A	429	GLU	3.8
1	A	213	LEU	3.7
1	A	35	PHE	3.7
1	A	18	LEU	3.7
1	A	43	PHE	3.7
1	A	294	GLY	3.7
1	A	95	LYS	3.6
1	A	204	GLU	3.5
1	A	326	ASP	3.5
1	A	60	LEU	3.5
1	A	226	LEU	3.5
1	A	392	PHE	3.4
1	A	445	LEU	3.4
1	A	402	ASN	3.3
1	A	299	ARG	3.3
1	A	321	ARG	3.3
1	A	372	GLN	3.2
1	A	152	TYR	3.2
1	A	300	ALA	3.1
1	A	144	ALA	3.1
1	A	223	GLU	3.0
1	A	41	LYS	3.0
1	A	12	ARG	2.9
1	A	425	LEU	2.9
1	A	38	LEU	2.7
1	A	438	CYS	2.7
1	A	419	LYS	2.7
1	A	208	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	34	ARG	2.7
1	A	88	LEU	2.6
1	A	14	THR	2.6
1	A	349	THR	2.6
1	A	262	ARG	2.5
1	A	80	ALA	2.5
1	A	364	LYS	2.5
1	A	104	THR	2.5
1	A	56	ASP	2.5
1	A	192	VAL	2.4
1	A	417	LYS	2.3
1	A	335	ARG	2.3
1	A	233	SER	2.3
1	A	433	HIS	2.3
1	A	13	GLN	2.2
1	A	377	GLY	2.2
1	A	146	TYR	2.2
1	A	437	HIS	2.2
1	A	190	LEU	2.2
1	A	427	ASN	2.2
1	A	98	VAL	2.2
1	A	175	ILE	2.1
1	A	78	HIS	2.1
1	A	261	ASP	2.1
1	A	366	ALA	2.1
1	A	352	GLY	2.0
1	A	272	THR	2.0
1	A	68	GLN	2.0
1	A	48	VAL	2.0
1	A	381	TRP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.