



# Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 02:21 PM EDT

PDB ID : 2YXQ / pdb\_00002yxq  
Title : The plug domain of the SecY protein stabilizes the closed state of the translocation channel and maintains a membrane seal  
Authors : Li, W.; Schulman, S.  
Deposited on : 2007-04-27  
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

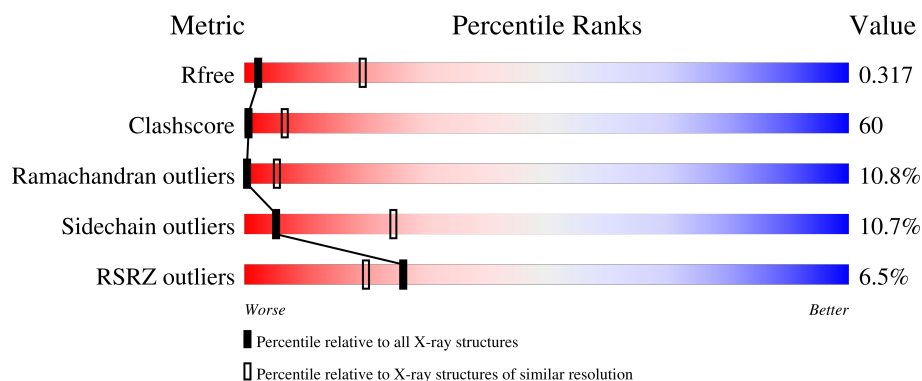
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	431	 7% 23% 59% 16% ..
2	B	74	 4% 26% 47% 14% • 12%
3	C	53	 21% 34% • • 40%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4052 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 Preprotein translocase subunit secY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3271	2187	515	550	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP Q60175
A	?	-	THR	deletion	UNP Q60175
A	?	-	ILE	deletion	UNP Q60175
A	?	-	THR	deletion	UNP Q60175
A	?	-	ALA	deletion	UNP Q60175
A	65	GLY	SER	SEE REMARK 999	UNP Q60175

- Molecule 2 is a protein called Preprotein translocase subunit secE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	65	Total	C	N	O	S	0	0	0
			524	348	85	90	1			

- Molecule 3 is a protein called Preprotein translocase secG subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	32	Total	C	N	O	0	0	0
			257	172	42	43			

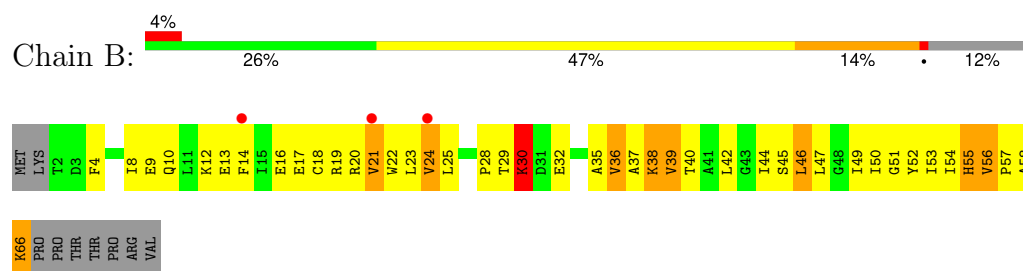
### 3 Residue-property plots [i](#)

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 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.

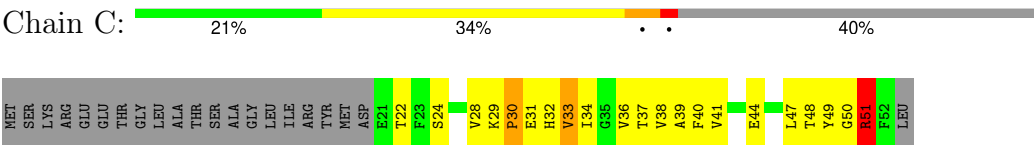
#### • Molecule 1: Preprotein translocase subunit secY



#### • Molecule 2: Preprotein translocase subunit secE



● Molecule 3: Preprotein translocase secG subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.23Å 148.49Å 81.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	70.6 (50.00-3.50) 70.5 (50.00-3.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.13 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.301 , 0.317 0.308 , 0.317	Depositor DCC
$R_{free}$ test set	538 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	146.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 175.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.69	0/3345	1.02	11/4540 (0.2%)
2	B	0.69	0/533	1.02	1/719 (0.1%)
3	C	0.67	0/262	1.00	2/354 (0.6%)
All	All	0.69	0/4140	1.02	14/5613 (0.2%)

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASP	CA-C-N	7.52	129.24	119.84
1	A	341	ASP	C-N-CA	7.52	129.24	119.84
1	A	334	TRP	N-CA-C	-7.47	104.32	113.50
1	A	375	PRO	N-CA-C	6.94	119.16	110.70
1	A	415	TYR	N-CA-C	-6.61	103.34	111.40
1	A	289	GLY	N-CA-C	-6.22	106.56	115.64
2	B	60	TYR	N-CA-C	-6.06	104.74	111.71
1	A	43	ILE	N-CA-C	6.06	117.30	108.58
1	A	394	PHE	N-CA-C	-6.04	104.61	111.07
3	C	29	LYS	CA-C-N	5.41	126.60	119.84
3	C	29	LYS	C-N-CA	5.41	126.60	119.84
1	A	117	ILE	N-CA-C	-5.39	104.63	110.23
1	A	129	ALA	N-CA-C	-5.15	106.77	113.16
1	A	39	ILE	O-C-N	-5.01	117.00	121.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	ARG	Mainchain

## 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	3271	0	3483	449	0
2	B	524	0	567	57	0
3	C	257	0	272	33	0
All	All	4052	0	4322	503	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 60.

All (503) 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:84:ILE:HD12	1:A:114:LEU:HD21	1.27	1.13
1:A:11:ILE:HD11	1:A:113:LEU:HD23	1.32	1.09
1:A:52:ILE:O	1:A:53:PRO:O	1.81	0.98
1:A:16:LEU:HD23	1:A:16:LEU:H	1.27	0.97
1:A:189:PRO:HD3	2:B:56:VAL:HG22	1.47	0.97
1:A:29:TRP:O	1:A:32:ILE:HG22	1.65	0.96
1:A:345:MET:O	1:A:349:ILE:HG13	1.64	0.96
1:A:157:LEU:HD23	1:A:160:ILE:HD12	1.49	0.94
1:A:426:LEU:O	1:A:428:PRO:HD3	1.68	0.91
1:A:124:VAL:HG22	1:A:144:ILE:HD13	1.51	0.91
1:A:240:ILE:HG22	1:A:241:LYS:H	1.34	0.90
1:A:314:ILE:HD12	1:A:315:HIS:H	1.37	0.90
1:A:67:ILE:HA	1:A:72:THR:HG23	1.53	0.90
1:A:287:TYR:HA	1:A:292:ALA:HA	1.53	0.90
1:A:52:ILE:O	1:A:53:PRO:C	2.15	0.88
1:A:13:GLU:HG3	1:A:14:VAL:H	1.36	0.87
1:A:98:LEU:HA	1:A:103:ASN:HB2	1.55	0.86
1:A:43:ILE:O	1:A:70:LEU:HD13	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HB3	1:A:209:TYR:CD2	2.12	0.84
1:A:3:LYS:HE3	1:A:3:LYS:HA	1.61	0.82
1:A:223:VAL:HG11	1:A:405:LEU:HA	1.58	0.82
1:A:393:ASN:HD21	1:A:402:THR:H	1.23	0.81
1:A:157:LEU:O	1:A:161:VAL:HG23	1.82	0.80
1:A:52:ILE:O	1:A:52:ILE:HG13	1.81	0.80
1:A:234:PRO:HB2	1:A:357:LYS:CB	2.10	0.80
1:A:388:LEU:O	1:A:391:ILE:HG22	1.83	0.79
2:B:58:ALA:O	2:B:62:LYS:HG3	1.81	0.79
1:A:317:ILE:O	1:A:321:ILE:HG13	1.83	0.79
1:A:75:ILE:HG22	1:A:79:VAL:HG23	1.64	0.78
1:A:152:ILE:HD13	1:A:155:ILE:HD12	1.63	0.78
1:A:228:CYS:SG	2:B:36:VAL:HG21	2.24	0.78
1:A:374:ILE:HB	1:A:375:PRO:HD3	1.65	0.77
1:A:102:GLU:O	1:A:106:LEU:HG	1.84	0.77
1:A:234:PRO:HB2	1:A:357:LYS:HB2	1.67	0.77
1:A:227:GLU:HA	1:A:252:VAL:HG21	1.66	0.77
1:A:72:THR:HB	1:A:147:ILE:HD12	1.64	0.77
1:A:33:VAL:HG13	1:A:157:LEU:HD22	1.66	0.76
1:A:53:PRO:HB2	1:A:55:ILE:HB	1.67	0.75
1:A:49:GLY:C	1:A:51:GLN:H	1.94	0.75
1:A:123:ALA:HB2	1:A:148:ALA:HB2	1.69	0.75
1:A:53:PRO:C	1:A:55:ILE:H	1.94	0.74
2:B:52:TYR:CE1	2:B:56:VAL:HG21	2.23	0.74
1:A:98:LEU:HA	1:A:103:ASN:CB	2.18	0.73
1:A:67:ILE:HG13	1:A:67:ILE:O	1.87	0.73
1:A:231:VAL:HB	1:A:249:ILE:CG1	2.20	0.72
2:B:16:GLU:O	2:B:20:ARG:HD3	1.89	0.72
3:C:36:VAL:O	3:C:39:ALA:HB3	1.88	0.72
1:A:356:ILE:HG22	1:A:357:LYS:H	1.54	0.71
1:A:82:GLY:HA2	1:A:111:GLN:NE2	2.04	0.71
1:A:257:ILE:HG21	1:A:334:TRP:CH2	2.25	0.71
3:C:34:ILE:O	3:C:38:VAL:HG23	1.91	0.70
1:A:231:VAL:HB	1:A:249:ILE:HG13	1.73	0.70
2:B:66:LYS:HB2	2:B:66:LYS:NZ	2.07	0.70
1:A:257:ILE:HG22	1:A:258:PRO:HD3	1.73	0.69
1:A:253:TYR:HE1	1:A:413:ARG:HH11	1.40	0.69
1:A:46:TYR:HB3	1:A:146:GLN:HE22	1.57	0.69
1:A:33:VAL:HG21	1:A:161:VAL:HG22	1.73	0.69
1:A:373:TYR:O	1:A:376:PRO:HG2	1.93	0.69
1:A:73:LEU:HD21	1:A:122:GLU:HB2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:THR:O	1:A:411:VAL:HG23	1.93	0.68
1:A:160:ILE:HD13	3:C:34:ILE:HD11	1.75	0.68
1:A:16:LEU:HD23	1:A:16:LEU:N	2.04	0.68
1:A:250:LYS:O	1:A:254:VAL:HG12	1.94	0.68
1:A:360:ARG:HB3	1:A:365:ALA:HB1	1.74	0.68
1:A:216:THR:HA	1:A:397:ALA:HB1	1.75	0.68
1:A:355:ALA:HB2	1:A:361:LYS:HA	1.74	0.68
2:B:21:VAL:C	2:B:23:LEU:H	2.02	0.68
1:A:13:GLU:HG3	1:A:14:VAL:N	2.09	0.67
1:A:35:VAL:HG13	2:B:54:ILE:HD11	1.74	0.67
1:A:230:ARG:HD3	1:A:248:PRO:HB2	1.75	0.67
1:A:84:ILE:CD1	1:A:114:LEU:HD21	2.18	0.67
1:A:274:LEU:HD13	1:A:274:LEU:O	1.95	0.67
1:A:53:PRO:C	1:A:55:ILE:N	2.47	0.67
1:A:164:TYR:CZ	3:C:30:PRO:HG2	2.30	0.67
1:A:80:THR:HG23	1:A:268:ASN:ND2	2.09	0.66
1:A:152:ILE:HD13	1:A:155:ILE:CD1	2.25	0.66
1:A:362:SER:HB2	1:A:365:ALA:HB2	1.77	0.66
1:A:129:ALA:HB1	1:A:274:LEU:HD12	1.78	0.65
1:A:93:ILE:HG22	1:A:94:ILE:HG13	1.79	0.65
1:A:188:GLY:HA2	2:B:52:TYR:HE1	1.60	0.65
1:A:273:GLY:HA3	1:A:287:TYR:OH	1.95	0.65
1:A:30:THR:O	1:A:33:VAL:HG23	1.96	0.65
1:A:219:VAL:O	1:A:223:VAL:HG23	1.97	0.65
1:A:333:PHE:O	1:A:337:THR:HG22	1.96	0.65
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.60	0.65
1:A:65:GLY:O	1:A:66:ARG:HG2	1.98	0.64
1:A:149:PHE:HD2	3:C:40:PHE:HZ	1.44	0.64
1:A:88:LEU:C	1:A:90:GLY:H	2.04	0.64
1:A:112:LYS:O	1:A:116:ILE:HD12	1.97	0.64
1:A:393:ASN:HD21	1:A:402:THR:N	1.95	0.63
1:A:146:GLN:HG2	3:C:44:GLU:OE1	1.98	0.63
1:A:254:VAL:HG22	1:A:255:SER:N	2.11	0.63
3:C:44:GLU:HA	3:C:47:LEU:HB3	1.81	0.63
1:A:103:ASN:HA	1:A:106:LEU:HD12	1.79	0.63
1:A:129:ALA:O	1:A:278:ARG:HD3	1.98	0.63
1:A:264:ALA:O	1:A:267:ALA:HB3	1.99	0.63
1:A:53:PRO:HG2	1:A:56:PHE:HD1	1.64	0.63
1:A:231:VAL:O	1:A:249:ILE:HG12	1.98	0.63
1:A:314:ILE:CD1	1:A:315:HIS:H	2.10	0.63
1:A:82:GLY:HA2	1:A:111:GLN:HE21	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ILE:N	1:A:281:ILE:HD12	2.14	0.63
1:A:338:THR:HG22	1:A:339:GLY:N	2.13	0.63
1:A:166:ILE:HG22	1:A:167:GLY:H	1.64	0.62
1:A:320:MET:O	1:A:324:ILE:HG12	1.99	0.62
1:A:195:LYS:HD3	1:A:209:TYR:HE2	1.63	0.62
1:A:254:VAL:HG22	1:A:381:SER:OG	1.99	0.62
2:B:4:PHE:O	2:B:8:ILE:HG13	1.99	0.62
2:B:55:HIS:O	2:B:56:VAL:C	2.42	0.62
2:B:46:LEU:HD11	2:B:50:ILE:HD11	1.82	0.62
1:A:79:VAL:O	1:A:83:ILE:HG13	2.00	0.61
1:A:279:MET:O	1:A:279:MET:HG2	2.00	0.61
1:A:362:SER:HB2	1:A:365:ALA:CB	2.31	0.61
1:A:84:ILE:O	1:A:87:LEU:HB2	2.00	0.61
1:A:425:GLU:O	1:A:426:LEU:HD12	2.01	0.61
1:A:5:ILE:N	1:A:6:PRO:HD2	2.16	0.61
1:A:257:ILE:HG21	1:A:334:TRP:CZ2	2.35	0.61
1:A:65:GLY:C	1:A:66:ARG:HG2	2.25	0.60
1:A:255:SER:HA	1:A:258:PRO:HG2	1.83	0.60
1:A:86:GLN:O	1:A:333:PHE:HD2	1.84	0.60
1:A:406:LEU:O	1:A:410:ILE:HG13	2.01	0.60
1:A:200:LEU:HD23	1:A:205:PRO:HG3	1.83	0.60
1:A:251:PHE:CE1	1:A:381:SER:HA	2.37	0.60
1:A:98:LEU:O	1:A:99:SER:C	2.43	0.60
1:A:342:PRO:HG3	1:A:374:ILE:CD1	2.31	0.60
1:A:240:ILE:HG22	1:A:241:LYS:N	2.10	0.60
1:A:36:LEU:O	1:A:40:MET:HG3	2.02	0.60
1:A:108:GLN:O	1:A:109:GLY:C	2.45	0.59
1:A:393:ASN:HD21	1:A:402:THR:HG22	1.66	0.59
1:A:3:LYS:C	1:A:5:ILE:H	2.10	0.59
1:A:211:ALA:HA	1:A:214:ILE:HD12	1.83	0.59
1:A:4:LEU:C	1:A:6:PRO:HD2	2.27	0.59
1:A:314:ILE:O	1:A:318:VAL:HG23	2.03	0.59
1:A:56:PHE:HD2	1:A:59:TRP:CE3	2.21	0.59
1:A:374:ILE:CB	1:A:375:PRO:HD3	2.32	0.59
1:A:179:SER:OG	2:B:44:ILE:HG23	2.01	0.59
1:A:94:ILE:O	1:A:94:ILE:HG22	2.03	0.59
1:A:274:LEU:HD13	1:A:274:LEU:C	2.28	0.59
1:A:273:GLY:CA	1:A:284:LEU:HD12	2.33	0.58
2:B:49:ILE:O	2:B:52:TYR:HB3	2.03	0.58
1:A:257:ILE:HG22	1:A:258:PRO:CD	2.33	0.58
1:A:189:PRO:C	1:A:191:GLY:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:C	1:A:241:LYS:HG3	2.29	0.58
1:A:5:ILE:HG22	1:A:9:GLU:CD	2.28	0.58
1:A:135:LEU:H	1:A:135:LEU:HD12	1.68	0.58
1:A:149:PHE:HB3	3:C:40:PHE:CZ	2.39	0.58
1:A:231:VAL:HB	1:A:249:ILE:HD11	1.84	0.58
1:A:254:VAL:CG2	1:A:255:SER:N	2.67	0.58
1:A:251:PHE:O	1:A:254:VAL:HG13	2.03	0.58
1:A:317:ILE:CG2	1:A:321:ILE:HD11	2.34	0.58
1:A:87:LEU:HD21	1:A:329:MET:HE1	1.84	0.58
1:A:166:ILE:HG22	1:A:167:GLY:N	2.19	0.58
1:A:100:ILE:HG22	1:A:102:GLU:H	1.67	0.57
1:A:256:ASN:N	1:A:258:PRO:HD2	2.19	0.57
1:A:311:SER:O	1:A:312:ASP:CG	2.47	0.57
2:B:16:GLU:HA	2:B:16:GLU:OE2	2.04	0.57
1:A:225:TYR:C	1:A:225:TYR:CD2	2.82	0.57
1:A:244:VAL:HG12	1:A:245:GLY:N	2.19	0.57
1:A:167:GLY:HA2	1:A:417:GLN:NE2	2.20	0.57
1:A:268:ASN:O	1:A:272:TRP:HB2	2.05	0.57
2:B:20:ARG:O	2:B:23:LEU:HB2	2.03	0.57
1:A:11:ILE:HD11	1:A:113:LEU:CD2	2.22	0.57
1:A:164:TYR:CE1	3:C:30:PRO:HG2	2.39	0.57
1:A:256:ASN:C	1:A:258:PRO:HD2	2.30	0.57
1:A:149:PHE:HB3	3:C:40:PHE:CE2	2.39	0.57
1:A:83:ILE:HG21	1:A:265:LEU:HD23	1.86	0.56
1:A:211:ALA:HB3	1:A:212:PRO:CD	2.35	0.56
1:A:231:VAL:HB	1:A:249:ILE:CD1	2.34	0.56
1:A:253:TYR:OH	1:A:413:ARG:HD2	2.05	0.56
1:A:384:PHE:O	1:A:387:PHE:HB3	2.05	0.56
2:B:36:VAL:O	2:B:37:ALA:C	2.47	0.56
1:A:98:LEU:O	1:A:100:ILE:N	2.38	0.56
1:A:342:PRO:HG3	1:A:374:ILE:HD11	1.87	0.56
1:A:75:ILE:HG22	1:A:79:VAL:CG2	2.32	0.56
1:A:23:PHE:HE1	1:A:421:GLU:HB2	1.70	0.56
1:A:328:VAL:HG12	1:A:332:ILE:HD11	1.87	0.56
1:A:129:ALA:C	1:A:278:ARG:HD3	2.31	0.56
1:A:317:ILE:HD12	1:A:317:ILE:H	1.71	0.56
1:A:153:ILE:HD11	3:C:40:PHE:CD1	2.40	0.56
1:A:171:GLY:O	1:A:410:ILE:HG21	2.06	0.56
1:A:257:ILE:N	1:A:258:PRO:CD	2.69	0.56
1:A:153:ILE:HD13	3:C:37:THR:HG23	1.87	0.56
1:A:327:CYS:O	1:A:328:VAL:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:HD23	1:A:8:LEU:C	2.31	0.55
1:A:139:LEU:O	1:A:143:VAL:HG23	2.05	0.55
1:A:344:SER:C	1:A:346:ALA:N	2.63	0.55
1:A:16:LEU:H	1:A:16:LEU:CD2	2.09	0.55
1:A:125:LEU:HD21	1:A:272:TRP:CD1	2.41	0.55
1:A:23:PHE:CD1	1:A:421:GLU:HB3	2.42	0.55
1:A:59:TRP:CD1	1:A:59:TRP:C	2.85	0.55
1:A:304:TYR:HD1	1:A:305:GLY:N	2.04	0.55
1:A:138:LEU:O	1:A:142:LEU:HG	2.05	0.55
1:A:224:VAL:O	1:A:225:TYR:C	2.48	0.55
1:A:49:GLY:C	1:A:51:GLN:N	2.60	0.55
1:A:255:SER:C	1:A:258:PRO:HD2	2.32	0.55
1:A:195:LYS:HD3	1:A:209:TYR:CE2	2.42	0.55
1:A:423:VAL:C	1:A:425:GLU:H	2.14	0.55
2:B:9:GLU:O	2:B:13:GLU:HG3	2.06	0.55
1:A:88:LEU:C	1:A:90:GLY:N	2.64	0.55
1:A:247:TYR:CD1	1:A:247:TYR:C	2.85	0.55
1:A:344:SER:O	1:A:346:ALA:N	2.40	0.55
1:A:75:ILE:HD11	1:A:173:PHE:CD1	2.42	0.54
1:A:328:VAL:O	1:A:332:ILE:HG13	2.07	0.54
1:A:59:TRP:O	1:A:65:GLY:C	2.50	0.54
1:A:273:GLY:HA2	1:A:284:LEU:HD12	1.89	0.54
1:A:400:GLY:O	1:A:401:GLY:C	2.50	0.54
1:A:56:PHE:O	1:A:59:TRP:HB3	2.07	0.54
2:B:21:VAL:O	2:B:23:LEU:N	2.41	0.54
1:A:80:THR:O	1:A:83:ILE:HB	2.08	0.54
1:A:43:ILE:HB	1:A:70:LEU:HD22	1.90	0.54
1:A:91:SER:C	1:A:93:ILE:H	2.16	0.54
1:A:29:TRP:NE1	1:A:164:TYR:HD2	2.06	0.53
1:A:82:GLY:O	1:A:86:GLN:HG2	2.07	0.53
1:A:216:THR:O	1:A:217:ILE:C	2.51	0.53
1:A:157:LEU:HA	1:A:160:ILE:HD12	1.90	0.53
1:A:334:TRP:O	1:A:337:THR:O	2.27	0.53
1:A:35:VAL:HG13	2:B:54:ILE:CD1	2.38	0.53
1:A:116:ILE:HA	1:A:119:CYS:HB2	1.91	0.53
1:A:237:HIS:HA	1:A:244:VAL:HG21	1.90	0.53
1:A:308:SER:HB3	1:A:394:PHE:O	2.09	0.53
1:A:66:ARG:O	1:A:67:ILE:HG12	2.09	0.53
1:A:160:ILE:HD13	3:C:34:ILE:CD1	2.39	0.53
1:A:287:TYR:CE2	1:A:292:ALA:HB2	2.43	0.53
1:A:405:LEU:O	1:A:406:LEU:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:TYR:CE1	2:B:56:VAL:CG2	2.92	0.53
1:A:166:ILE:HD13	1:A:418:LEU:CD2	2.38	0.52
1:A:14:VAL:HG21	1:A:159:GLU:HB3	1.91	0.52
1:A:169:GLY:O	1:A:170:ILE:C	2.52	0.52
1:A:172:LEU:HD23	1:A:176:ALA:HB2	1.91	0.52
1:A:102:GLU:C	1:A:106:LEU:HG	2.35	0.52
1:A:160:ILE:HD11	3:C:33:VAL:CG2	2.40	0.52
1:A:231:VAL:CG1	1:A:249:ILE:HD11	2.39	0.52
1:A:377:LEU:HA	2:B:21:VAL:HG11	1.90	0.52
3:C:22:THR:HG22	3:C:24:SER:H	1.74	0.52
1:A:53:PRO:HB2	1:A:55:ILE:CB	2.40	0.52
1:A:35:VAL:O	1:A:36:LEU:C	2.49	0.52
1:A:260:ILE:HG12	1:A:406:LEU:HD13	1.91	0.52
1:A:317:ILE:HG23	1:A:321:ILE:HD11	1.91	0.52
1:A:325:ILE:HG13	1:A:326:THR:N	2.24	0.52
1:A:85:MET:HE2	1:A:111:GLN:HB2	1.92	0.51
1:A:270:GLN:NE2	1:A:301:SER:HB3	2.25	0.51
1:A:89:VAL:HG21	1:A:107:PHE:CD1	2.46	0.51
1:A:166:ILE:O	1:A:167:GLY:C	2.53	0.51
1:A:247:TYR:C	1:A:247:TYR:HD1	2.17	0.51
1:A:306:LEU:N	1:A:306:LEU:HD12	2.26	0.51
1:A:151:SER:O	1:A:155:ILE:HG13	2.10	0.51
1:A:332:ILE:O	1:A:335:VAL:HB	2.10	0.51
1:A:53:PRO:O	1:A:55:ILE:N	2.43	0.51
1:A:195:LYS:O	1:A:199:SER:HB2	2.11	0.51
1:A:425:GLU:O	1:A:425:GLU:HG3	2.10	0.51
1:A:350:GLY:O	1:A:353:GLY:N	2.43	0.51
1:A:98:LEU:O	1:A:100:ILE:O	2.29	0.51
2:B:29:THR:O	2:B:32:GLU:N	2.43	0.51
1:A:143:VAL:O	1:A:144:ILE:C	2.53	0.51
1:A:402:THR:O	1:A:405:LEU:HB3	2.11	0.51
1:A:230:ARG:HG3	1:A:230:ARG:NH1	2.26	0.51
1:A:135:LEU:HD12	1:A:135:LEU:N	2.26	0.50
1:A:172:LEU:CD2	1:A:176:ALA:HB2	2.40	0.50
1:A:180:GLN:HG3	2:B:51:GLY:HA3	1.93	0.50
1:A:223:VAL:CG1	1:A:405:LEU:HA	2.36	0.50
1:A:423:VAL:C	1:A:425:GLU:N	2.65	0.50
1:A:225:TYR:C	1:A:225:TYR:HD2	2.19	0.50
1:A:342:PRO:HA	1:A:345:MET:HB2	1.93	0.50
1:A:385:VAL:O	1:A:386:GLY:C	2.53	0.50
2:B:45:SER:O	2:B:46:LEU:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ALA:O	3:C:40:PHE:C	2.54	0.50
1:A:67:ILE:O	1:A:67:ILE:CG1	2.58	0.50
1:A:429:ALA:O	1:A:431:ALA:N	2.41	0.50
1:A:18:VAL:HG12	1:A:18:VAL:O	2.12	0.50
1:A:265:LEU:HD13	1:A:265:LEU:C	2.37	0.50
1:A:355:ALA:O	1:A:356:ILE:O	2.29	0.50
1:A:359:PHE:O	1:A:360:ARG:HB2	2.12	0.50
1:A:34:LEU:O	1:A:37:TYR:HB3	2.12	0.49
2:B:66:LYS:HB2	2:B:66:LYS:HZ2	1.77	0.49
1:A:314:ILE:HD12	1:A:315:HIS:N	2.18	0.49
1:A:344:SER:C	1:A:346:ALA:H	2.20	0.49
1:A:22:THR:OG1	1:A:25:GLU:HG3	2.12	0.49
1:A:53:PRO:HG2	1:A:56:PHE:CD1	2.46	0.49
1:A:304:TYR:CD1	1:A:304:TYR:C	2.90	0.49
1:A:167:GLY:HA2	1:A:417:GLN:CD	2.37	0.49
1:A:356:ILE:HG22	1:A:357:LYS:N	2.24	0.49
1:A:410:ILE:O	1:A:414:MET:HB2	2.12	0.49
1:A:23:PHE:HD1	1:A:421:GLU:HB3	1.77	0.49
1:A:112:LYS:HD3	1:A:116:ILE:HD11	1.94	0.49
1:A:388:LEU:HD23	1:A:405:LEU:CD1	2.42	0.49
1:A:118:MET:HE3	1:A:122:GLU:HG2	1.94	0.48
1:A:331:GLY:O	1:A:334:TRP:HB3	2.12	0.48
1:A:374:ILE:HB	1:A:375:PRO:CD	2.41	0.48
2:B:8:ILE:O	2:B:12:LYS:HG3	2.13	0.48
1:A:236:ALA:CB	1:A:355:ALA:O	2.61	0.48
1:A:256:ASN:C	1:A:258:PRO:CD	2.85	0.48
1:A:362:SER:O	1:A:365:ALA:HB3	2.13	0.48
1:A:216:THR:HA	1:A:397:ALA:CB	2.43	0.48
1:A:340:LEU:O	1:A:342:PRO:HD3	2.14	0.48
3:C:37:THR:C	3:C:39:ALA:N	2.71	0.48
1:A:256:ASN:O	1:A:257:ILE:C	2.57	0.48
1:A:382:SER:O	1:A:383:ALA:C	2.56	0.48
2:B:66:LYS:HB2	2:B:66:LYS:HZ3	1.79	0.48
3:C:49:TYR:CD1	3:C:49:TYR:N	2.81	0.48
1:A:5:ILE:HG22	1:A:9:GLU:OE1	2.13	0.48
1:A:142:LEU:O	1:A:145:ILE:HB	2.13	0.48
1:A:203:GLY:C	1:A:205:PRO:HD3	2.39	0.48
1:A:153:ILE:HG21	3:C:37:THR:HG23	1.96	0.48
1:A:214:ILE:O	1:A:215:GLY:C	2.57	0.48
1:A:149:PHE:CD2	3:C:40:PHE:HZ	2.30	0.48
2:B:29:THR:O	2:B:30:LYS:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:CA	1:A:72:THR:HG23	2.36	0.48
1:A:304:TYR:HB3	1:A:393:ASN:O	2.14	0.48
1:A:379:VAL:O	1:A:380:MET:C	2.56	0.48
1:A:234:PRO:C	1:A:357:LYS:HB2	2.39	0.47
2:B:32:GLU:O	2:B:35:ALA:HB3	2.15	0.47
1:A:152:ILE:HA	1:A:155:ILE:CD1	2.43	0.47
2:B:35:ALA:O	2:B:38:LYS:HB2	2.15	0.47
1:A:163:LYS:O	1:A:164:TYR:CD1	2.68	0.47
1:A:316:ALA:O	1:A:317:ILE:C	2.56	0.47
1:A:385:VAL:HG12	1:A:386:GLY:N	2.28	0.47
2:B:53:ILE:O	2:B:57:PRO:HG3	2.14	0.47
1:A:149:PHE:O	1:A:152:ILE:HB	2.15	0.47
1:A:153:ILE:HD13	3:C:37:THR:HA	1.96	0.47
1:A:206:ASN:HB3	1:A:209:TYR:HD1	1.79	0.47
1:A:304:TYR:CD1	1:A:305:GLY:N	2.83	0.47
1:A:337:THR:O	1:A:338:THR:C	2.56	0.47
1:A:374:ILE:HG22	1:A:375:PRO:N	2.29	0.47
1:A:77:PRO:O	1:A:78:ILE:C	2.58	0.47
1:A:152:ILE:HA	1:A:155:ILE:HD12	1.97	0.47
1:A:343:LYS:O	1:A:346:ALA:HB3	2.14	0.47
3:C:32:HIS:O	3:C:36:VAL:HG23	2.15	0.47
1:A:156:TYR:O	1:A:160:ILE:HG13	2.14	0.47
1:A:415:TYR:CG	2:B:39:VAL:HG21	2.50	0.47
2:B:23:LEU:C	2:B:25:LEU:H	2.23	0.47
1:A:89:VAL:HG12	1:A:89:VAL:O	2.15	0.47
1:A:33:VAL:CG1	1:A:157:LEU:HD22	2.40	0.47
1:A:240:ILE:O	1:A:241:LYS:HG3	2.14	0.47
1:A:8:LEU:HD23	1:A:8:LEU:O	2.15	0.46
1:A:80:THR:HG21	1:A:118:MET:HE2	1.97	0.46
1:A:135:LEU:O	1:A:137:PRO:HD3	2.16	0.46
1:A:130:GLY:HA3	1:A:278:ARG:CZ	2.45	0.46
1:A:342:PRO:CG	1:A:374:ILE:HD12	2.45	0.46
2:B:46:LEU:O	2:B:47:LEU:C	2.58	0.46
1:A:172:LEU:CD2	1:A:172:LEU:C	2.88	0.46
3:C:30:PRO:O	3:C:31:GLU:C	2.59	0.46
1:A:45:VAL:HG11	1:A:147:ILE:HD11	1.96	0.46
1:A:59:TRP:HD1	1:A:65:GLY:N	2.14	0.46
1:A:255:SER:OG	1:A:382:SER:HB3	2.15	0.46
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.81	0.46
1:A:374:ILE:O	1:A:377:LEU:HB3	2.16	0.46
1:A:228:CYS:HB2	2:B:28:PRO:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:GLY:O	3:C:51:ARG:C	2.59	0.46
1:A:139:LEU:HA	1:A:142:LEU:HD12	1.97	0.46
1:A:181:THR:HG21	1:A:399:GLY:HA2	1.98	0.46
2:B:18:CYS:HA	2:B:21:VAL:HG23	1.98	0.46
1:A:259:VAL:CG1	1:A:406:LEU:HD21	2.46	0.45
1:A:153:ILE:HG22	1:A:157:LEU:HD12	1.96	0.45
1:A:319:TYR:O	1:A:322:ALA:HB3	2.17	0.45
1:A:419:LEU:C	1:A:421:GLU:N	2.71	0.45
1:A:44:ASP:HB2	3:C:49:TYR:OH	2.16	0.45
1:A:179:SER:OG	2:B:44:ILE:CG2	2.65	0.45
1:A:260:ILE:HG12	1:A:406:LEU:CD1	2.45	0.45
1:A:388:LEU:O	1:A:389:ALA:C	2.59	0.45
1:A:169:GLY:O	1:A:172:LEU:HB3	2.16	0.45
1:A:172:LEU:HD23	1:A:172:LEU:C	2.40	0.45
1:A:384:PHE:O	1:A:385:VAL:C	2.59	0.45
1:A:374:ILE:CB	1:A:375:PRO:CD	2.94	0.45
1:A:148:ALA:O	1:A:152:ILE:HG12	2.16	0.45
1:A:389:ALA:O	1:A:390:THR:C	2.58	0.45
1:A:370:LEU:O	1:A:374:ILE:HG13	2.16	0.45
1:A:35:VAL:C	1:A:37:TYR:N	2.73	0.45
1:A:236:ALA:HB3	1:A:355:ALA:O	2.16	0.45
1:A:299:TYR:O	1:A:300:LEU:HD23	2.17	0.45
1:A:342:PRO:HG3	1:A:374:ILE:HD12	1.99	0.45
1:A:360:ARG:HH11	1:A:360:ARG:HG3	1.82	0.45
1:A:393:ASN:ND2	1:A:402:THR:HG22	2.30	0.45
2:B:24:VAL:HG12	2:B:24:VAL:O	2.16	0.45
1:A:88:LEU:O	1:A:90:GLY:N	2.50	0.45
1:A:423:VAL:O	1:A:425:GLU:N	2.50	0.44
1:A:112:LYS:HD3	1:A:116:ILE:CD1	2.48	0.44
1:A:293:VAL:O	1:A:293:VAL:HG12	2.16	0.44
1:A:332:ILE:HG13	1:A:332:ILE:H	1.66	0.44
1:A:359:PHE:O	1:A:360:ARG:CB	2.66	0.44
1:A:13:GLU:CG	1:A:14:VAL:H	2.17	0.44
1:A:38:PHE:CD1	2:B:50:ILE:HG22	2.51	0.44
1:A:108:GLN:O	1:A:110:CYS:N	2.50	0.44
1:A:136:THR:O	1:A:137:PRO:C	2.61	0.44
2:B:14:PHE:CD1	2:B:14:PHE:C	2.96	0.44
1:A:6:PRO:HG2	1:A:7:ILE:H	1.82	0.44
1:A:381:SER:O	1:A:384:PHE:HB3	2.18	0.44
1:A:75:ILE:HD11	1:A:173:PHE:HD1	1.82	0.44
1:A:405:LEU:C	1:A:405:LEU:HD23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:GLN:O	2:B:13:GLU:HB2	2.18	0.44
2:B:61:ILE:O	2:B:62:LYS:C	2.60	0.44
3:C:30:PRO:O	3:C:34:ILE:HG12	2.17	0.44
1:A:189:PRO:C	1:A:191:GLY:N	2.76	0.43
1:A:265:LEU:HD13	1:A:265:LEU:O	2.18	0.43
1:A:410:ILE:O	1:A:413:ARG:HG2	2.17	0.43
1:A:3:LYS:O	1:A:5:ILE:N	2.47	0.43
1:A:21:ILE:HD12	1:A:21:ILE:H	1.83	0.43
1:A:75:ILE:O	1:A:79:VAL:HG23	2.18	0.43
1:A:91:SER:OG	1:A:93:ILE:HG13	2.17	0.43
1:A:256:ASN:C	1:A:258:PRO:N	2.76	0.43
2:B:62:LYS:O	2:B:66:LYS:HB2	2.18	0.43
1:A:92:GLY:O	1:A:95:GLN:HG3	2.18	0.43
1:A:231:VAL:CB	1:A:249:ILE:HD11	2.47	0.43
1:A:277:TYR:C	1:A:279:MET:H	2.25	0.43
1:A:154:LEU:O	1:A:155:ILE:C	2.60	0.43
1:A:252:VAL:HG23	1:A:253:TYR:N	2.33	0.43
1:A:392:ALA:O	1:A:395:ILE:CG2	2.66	0.43
1:A:145:ILE:O	1:A:146:GLN:C	2.62	0.43
1:A:189:PRO:HD3	2:B:56:VAL:CG2	2.34	0.43
1:A:201:ILE:C	1:A:203:GLY:N	2.76	0.43
1:A:392:ALA:C	1:A:395:ILE:HG22	2.44	0.43
3:C:30:PRO:HA	3:C:33:VAL:CG2	2.48	0.43
1:A:302:THR:HA	1:A:303:PRO:HD3	1.83	0.43
1:A:92:GLY:O	1:A:94:ILE:N	2.51	0.43
1:A:240:ILE:CG2	1:A:241:LYS:N	2.78	0.43
1:A:411:VAL:O	1:A:414:MET:HB3	2.19	0.43
2:B:14:PHE:CE1	2:B:18:CYS:SG	3.12	0.43
1:A:12:PRO:HB3	3:C:28:VAL:HG21	2.00	0.43
1:A:98:LEU:HD23	1:A:103:ASN:HB3	1.99	0.43
2:B:35:ALA:O	2:B:36:VAL:C	2.61	0.43
1:A:56:PHE:HD2	1:A:59:TRP:HE3	1.61	0.42
1:A:83:ILE:HG23	1:A:330:PHE:CZ	2.53	0.42
1:A:86:GLN:O	1:A:90:GLY:HA3	2.18	0.42
1:A:322:ALA:O	1:A:326:THR:OG1	2.36	0.42
3:C:30:PRO:O	3:C:33:VAL:HG23	2.18	0.42
1:A:92:GLY:O	1:A:93:ILE:C	2.62	0.42
1:A:112:LYS:O	1:A:115:SER:HB3	2.18	0.42
1:A:188:GLY:HA2	2:B:52:TYR:CE1	2.48	0.42
1:A:244:VAL:HG12	1:A:245:GLY:H	1.83	0.42
1:A:287:TYR:CD2	1:A:292:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:VAL:HG13	2:B:40:THR:HG21	2.01	0.42
1:A:136:THR:HB	1:A:139:LEU:HB3	2.00	0.42
1:A:412:TYR:C	1:A:414:MET:N	2.77	0.42
1:A:427:HIS:O	1:A:429:ALA:N	2.52	0.42
1:A:52:ILE:O	1:A:52:ILE:CG1	2.59	0.42
1:A:38:PHE:CD1	2:B:51:GLY:HA2	2.54	0.42
1:A:43:ILE:HG22	1:A:70:LEU:HD11	2.02	0.42
1:A:146:GLN:HE21	3:C:44:GLU:CG	2.32	0.42
1:A:274:LEU:C	1:A:274:LEU:CD1	2.92	0.42
1:A:136:THR:O	1:A:138:LEU:N	2.52	0.42
1:A:238:GLY:O	1:A:239:ARG:HB2	2.19	0.42
1:A:250:LYS:O	1:A:254:VAL:CG1	2.65	0.42
1:A:253:TYR:CZ	1:A:413:ARG:HD2	2.54	0.42
1:A:194:TRP:O	1:A:195:LYS:C	2.63	0.42
1:A:206:ASN:CG	1:A:209:TYR:HD1	2.28	0.42
1:A:251:PHE:CE2	2:B:25:LEU:HD11	2.54	0.42
1:A:391:ILE:CG2	1:A:392:ALA:N	2.83	0.42
1:A:168:SER:O	1:A:172:LEU:HB2	2.20	0.42
1:A:197:LEU:HD13	1:A:197:LEU:HA	1.92	0.42
1:A:25:GLU:O	1:A:26:LYS:C	2.62	0.42
1:A:124:VAL:CG2	1:A:144:ILE:HD13	2.37	0.42
1:A:166:ILE:HD13	1:A:418:LEU:HD21	2.00	0.42
1:A:194:TRP:C	1:A:196:PHE:N	2.77	0.42
1:A:259:VAL:HG12	1:A:406:LEU:HD21	2.02	0.42
1:A:260:ILE:O	1:A:264:ALA:HB2	2.20	0.42
1:A:98:LEU:HD22	1:A:104:ARG:HA	2.02	0.41
1:A:194:TRP:O	1:A:196:PHE:N	2.53	0.41
1:A:312:ASP:N	1:A:313:PRO:HD3	2.35	0.41
1:A:24:LYS:O	1:A:28:LYS:HG3	2.20	0.41
1:A:370:LEU:C	1:A:372:ARG:N	2.78	0.41
1:A:388:LEU:HD23	1:A:405:LEU:HD12	2.01	0.41
2:B:40:THR:O	2:B:44:ILE:HG13	2.20	0.41
2:B:49:ILE:HG22	2:B:53:ILE:HD11	2.01	0.41
1:A:130:GLY:HA3	1:A:278:ARG:NH1	2.35	0.41
1:A:219:VAL:HG12	1:A:404:VAL:HG11	2.01	0.41
1:A:256:ASN:O	1:A:258:PRO:N	2.53	0.41
1:A:330:PHE:O	1:A:334:TRP:HB2	2.21	0.41
1:A:59:TRP:C	1:A:59:TRP:HD1	2.26	0.41
1:A:234:PRO:CB	1:A:357:LYS:HB2	2.43	0.41
1:A:363:GLU:C	1:A:365:ALA:N	2.76	0.41
1:A:387:PHE:O	1:A:388:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:CB	1:A:55:ILE:HD12	2.50	0.41
1:A:172:LEU:O	1:A:173:PHE:C	2.62	0.41
1:A:23:PHE:CE1	1:A:421:GLU:CB	3.04	0.41
1:A:70:LEU:N	1:A:70:LEU:CD1	2.84	0.41
1:A:74:GLY:O	1:A:77:PRO:HD2	2.21	0.41
1:A:170:ILE:H	1:A:170:ILE:HG13	1.41	0.41
1:A:310:ILE:O	1:A:313:PRO:HD3	2.21	0.41
1:A:39:ILE:O	1:A:40:MET:C	2.59	0.41
1:A:363:GLU:O	1:A:364:LYS:C	2.64	0.41
1:A:380:MET:HG2	2:B:18:CYS:O	2.20	0.41
1:A:14:VAL:HG21	1:A:159:GLU:CB	2.51	0.41
1:A:118:MET:O	1:A:122:GLU:CG	2.69	0.41
1:A:206:ASN:ND2	1:A:209:TYR:CE1	2.89	0.41
1:A:324:ILE:HD11	1:A:387:PHE:HB2	2.03	0.41
2:B:49:ILE:O	2:B:52:TYR:N	2.52	0.41
1:A:85:MET:HB3	1:A:107:PHE:CE1	2.57	0.40
1:A:100:ILE:C	1:A:102:GLU:N	2.77	0.40
1:A:132:PHE:CD1	1:A:132:PHE:N	2.90	0.40
1:A:234:PRO:HA	1:A:246:LYS:HA	2.02	0.40
3:C:32:HIS:O	3:C:33:VAL:C	2.63	0.40
1:A:314:ILE:CD1	1:A:315:HIS:N	2.82	0.40
1:A:355:ALA:CB	1:A:361:LYS:HA	2.48	0.40
2:B:21:VAL:C	2:B:23:LEU:N	2.67	0.40
1:A:129:ALA:O	1:A:274:LEU:HD11	2.22	0.40
1:A:170:ILE:O	1:A:171:GLY:C	2.64	0.40
1:A:240:ILE:CG2	1:A:241:LYS:H	2.11	0.40
1:A:421:GLU:O	1:A:422:LYS:C	2.65	0.40
2:B:57:PRO:O	2:B:60:TYR:N	2.55	0.40
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.90	0.40
1:A:146:GLN:HE21	3:C:44:GLU:HG2	1.86	0.40
1:A:166:ILE:HD13	1:A:418:LEU:HD23	2.04	0.40
1:A:232:GLU:O	1:A:233:ILE:HD13	2.22	0.40
1:A:344:SER:O	1:A:345:MET:C	2.65	0.40
3:C:48:THR:HB	3:C:49:TYR:CD1	2.57	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	425/431 (99%)	273 (64%)	105 (25%)	47 (11%)	0	5
2	B	63/74 (85%)	44 (70%)	12 (19%)	7 (11%)	0	5
3	C	30/53 (57%)	20 (67%)	8 (27%)	2 (7%)	1	11
All	All	518/558 (93%)	337 (65%)	125 (24%)	56 (11%)	0	5

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	PRO
1	A	99	SER
1	A	145	ILE
1	A	170	ILE
1	A	240	ILE
1	A	311	SER
1	A	338	THR
1	A	356	ILE
1	A	360	ARG
1	A	374	ILE
1	A	385	VAL
1	A	430	ILE
1	A	188	GLY
1	A	189	PRO
1	A	244	VAL
1	A	245	GLY
1	A	339	GLY
1	A	345	MET
1	A	346	ALA
1	A	396	GLY
2	B	22	TRP
2	B	24	VAL
3	C	51	ARG
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	93	ILE
1	A	190	GLU
1	A	205	PRO
1	A	304	TYR
1	A	329	MET
2	B	30	LYS
2	B	38	LYS
2	B	55	HIS
1	A	6	PRO
1	A	108	GLN
1	A	144	ILE
1	A	147	ILE
1	A	246	LYS
1	A	256	ASN
1	A	312	ASP
1	A	429	ALA
2	B	46	LEU
3	C	41	VAL
1	A	67	ILE
1	A	247	TYR
1	A	288	GLU
1	A	363	GLU
1	A	377	LEU
1	A	102	GLU
1	A	109	GLY
1	A	137	PRO
2	B	56	VAL
1	A	89	VAL
1	A	248	PRO
1	A	358	GLY
1	A	143	VAL
1	A	258	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	A	346/350 (99%)	311 (90%)	35 (10%)	6	26
2	B	57/66 (86%)	49 (86%)	8 (14%)	3	16
3	C	28/45 (62%)	25 (89%)	3 (11%)	5	24
All	All	431/461 (94%)	385 (89%)	46 (11%)	5	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	16	LEU
1	A	21	ILE
1	A	22	THR
1	A	27	LEU
1	A	33	VAL
1	A	51	GLN
1	A	112	LYS
1	A	126	PHE
1	A	135	LEU
1	A	161	VAL
1	A	170	ILE
1	A	172	LEU
1	A	197	LEU
1	A	202	GLN
1	A	205	PRO
1	A	210	ILE
1	A	213	ILE
1	A	219	VAL
1	A	248	PRO
1	A	254	VAL
1	A	257	ILE
1	A	259	VAL
1	A	306	LEU
1	A	309	VAL
1	A	314	ILE
1	A	326	THR
1	A	336	GLU
1	A	349	ILE
1	A	363	GLU
1	A	369	ARG
1	A	380	MET
1	A	381	SER
1	A	402	THR

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Mol	Chain	Res	Type
1	A	417	GLN
2	B	17	GLU
2	B	19	ARG
2	B	21	VAL
2	B	30	LYS
2	B	36	VAL
2	B	39	VAL
2	B	42	LEU
2	B	66	LYS
3	C	30	PRO
3	C	33	VAL
3	C	51	ARG

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

Mol	Chain	Res	Type
1	A	111	GLN
1	A	146	GLN
1	A	256	ASN
1	A	268	ASN
1	A	286	HIS
1	A	315	HIS
1	A	393	ASN
1	A	417	GLN
2	B	6	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 oligosaccharides in this entry.



## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	427/431 (99%)	0.37	31 (7%) 22 18	64, 153, 232, 251	0
2	B	65/74 (87%)	0.21	3 (4%) 38 27	94, 135, 223, 237	0
3	C	32/53 (60%)	0.32	0 100 100	104, 181, 206, 206	0
All	All	524/558 (93%)	0.35	34 (6%) 26 20	64, 153, 232, 251	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	GLY	5.9
1	A	289	GLY	5.5
1	A	12	PRO	5.4
1	A	398	LEU	5.2
1	A	11	ILE	4.9
1	A	427	HIS	3.8
1	A	309	VAL	3.6
1	A	340	LEU	3.5
1	A	360	ARG	3.4
1	A	323	MET	3.4
1	A	245	GLY	3.3
1	A	293	VAL	3.1
1	A	132	PHE	3.0
1	A	399	GLY	3.0
1	A	354	MET	2.9
1	A	359	PHE	2.9
1	A	283	ILE	2.8
2	B	24	VAL	2.7
1	A	347	LYS	2.7
1	A	115	SER	2.6
1	A	288	GLU	2.6
1	A	263	ALA	2.5
1	A	14	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	310	ILE	2.3
1	A	422	LYS	2.3
1	A	413	ARG	2.3
1	A	234	PRO	2.2
1	A	131	ALA	2.2
1	A	257	ILE	2.2
1	A	126	PHE	2.2
2	B	21	VAL	2.1
1	A	134	ILE	2.1
1	A	352	LEU	2.1
2	B	14	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.