



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:49 AM UTC

PDB ID : 2YXR / pdb_00002yxr
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 : 3.60 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

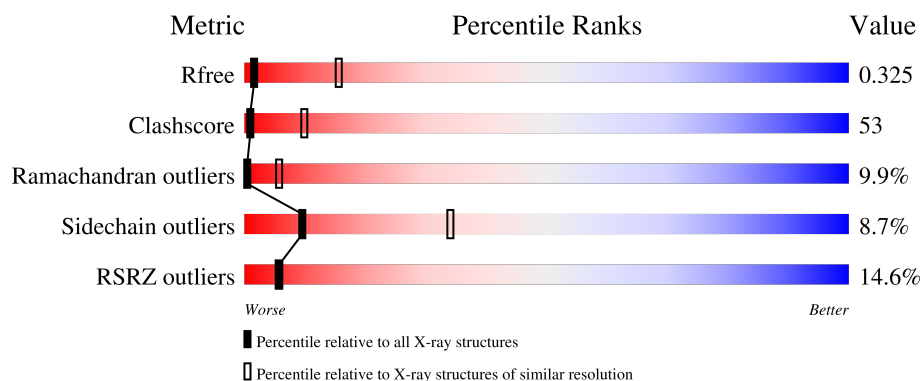
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. 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	426	17% 26% 59% 14%
2	B	74	3% 32% 46% 8% 12%
3	C	53	4% 21% 34% 6% 40%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3999 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	422	Total	C	N	O	S	0	0	0
			3218	2150	506	543	19			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q60175
A	?	-	PHE	deletion	UNP Q60175
A	?	-	TRP	deletion	UNP Q60175
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	?	-	SER	deletion	UNP Q60175
A	?	-	ARG	deletion	UNP Q60175
A	67	GLY	ILE	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			

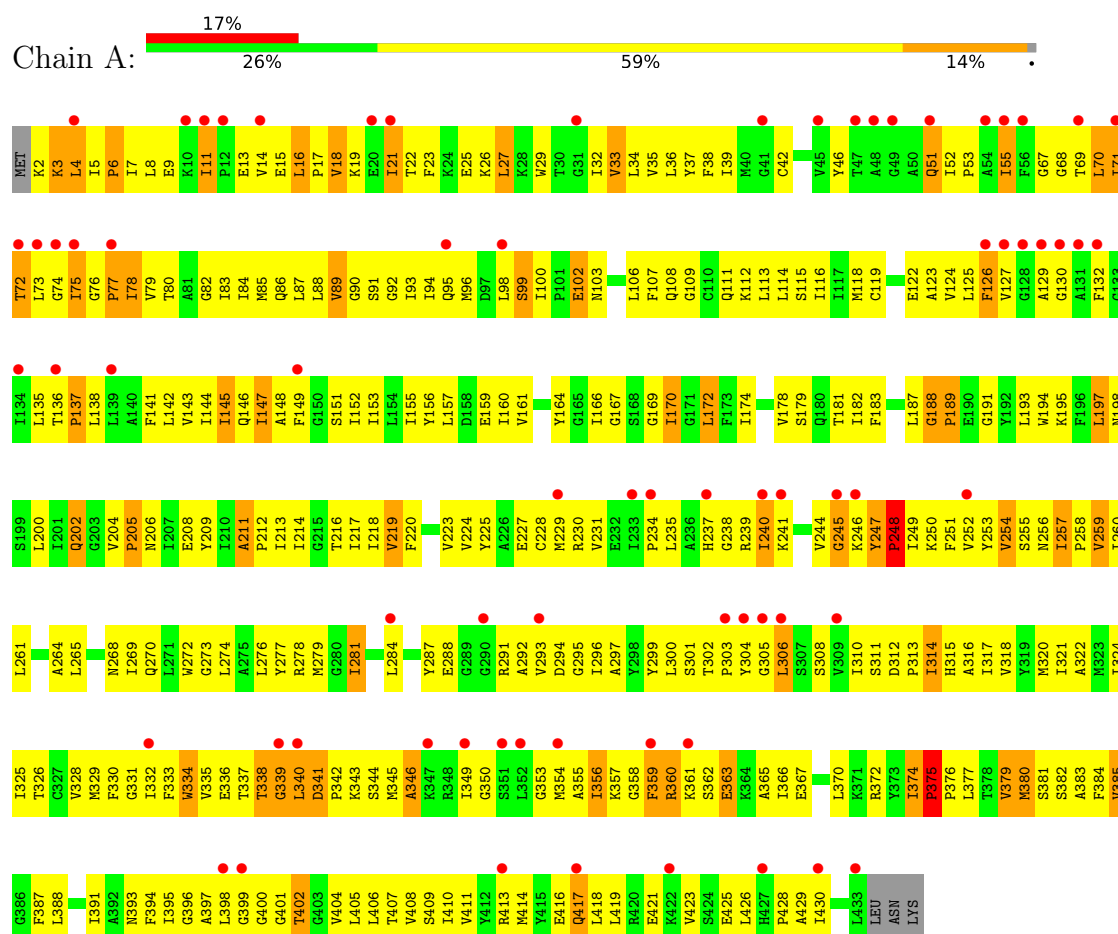
- Molecule 3 is a protein called Preprotein translocase secG subunit.

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

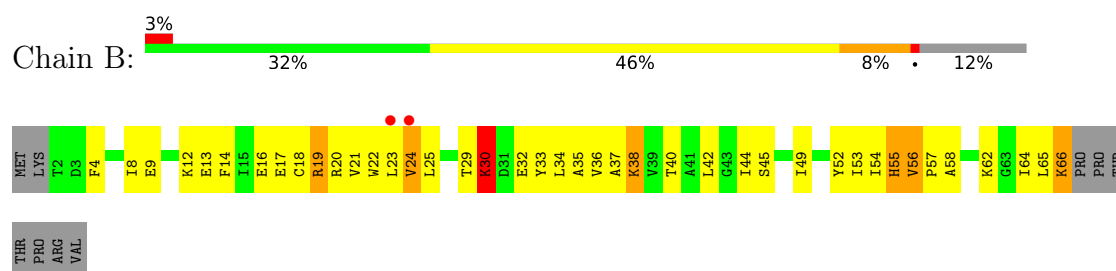
3 Residue-property plots [i](#)

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.

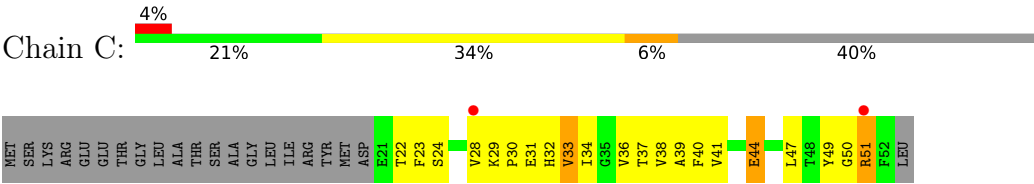
• Molecule 1: Preprotein translocase subunit secY



• 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, α , β , γ	92.51Å 150.36Å 79.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 3.60 44.07 – 3.60	Depositor EDS
% Data completeness (in resolution range)	65.7 (44.07-3.60) 65.6 (44.07-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.52 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.3.0026	Depositor
R, R_{free}	0.298 , 0.335 0.300 , 0.325	Depositor DCC
R_{free} test set	465 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	116.5	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 146.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3999	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.71	0/3289	1.00	6/4464 (0.1%)
2	B	0.72	0/533	0.93	0/719
3	C	0.60	0/262	0.93	2/354 (0.6%)
All	All	0.71	0/4084	0.98	8/5537 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASP	CA-C-N	6.78	127.04	119.32
1	A	341	ASP	C-N-CA	6.78	127.04	119.32
1	A	18	VAL	N-CA-C	-6.05	105.84	112.80
1	A	334	TRP	N-CA-C	-6.03	105.93	113.28
1	A	11	ILE	CA-C-N	5.26	125.55	119.92
1	A	11	ILE	C-N-CA	5.26	125.55	119.92
3	C	29	LYS	CA-C-N	5.22	126.37	119.84
3	C	29	LYS	C-N-CA	5.22	126.37	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3218	0	3434	392	0
2	B	524	0	567	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	257	0	272	32	0
All	All	3999	0	4273	439	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 53.

All (439) 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	1.38	1.01
1:A:29:TRP:O	1:A:32:ILE:HG22	1.62	0.99
1:A:11:ILE:HD11	1:A:113:LEU:HD23	1.43	0.97
1:A:16:LEU:HD23	1:A:16:LEU:H	1.30	0.96
1:A:240:ILE:HG22	1:A:241:LYS:H	1.31	0.93
1:A:340:LEU:H	1:A:340:LEU:HD12	1.38	0.88
1:A:33:VAL:HG21	1:A:161:VAL:HG22	1.56	0.88
1:A:227:GLU:HA	1:A:252:VAL:HG21	1.55	0.87
1:A:314:ILE:HD12	1:A:315:HIS:H	1.39	0.87
1:A:426:LEU:O	1:A:428:PRO:HD3	1.75	0.86
1:A:377:LEU:HA	2:B:21:VAL:HG11	1.57	0.86
1:A:13:GLU:HG3	1:A:14:VAL:H	1.42	0.85
1:A:287:TYR:HA	1:A:292:ALA:HA	1.58	0.83
1:A:46:TYR:HB3	1:A:146:GLN:HE22	1.41	0.83
1:A:200:LEU:HD23	1:A:205:PRO:HG3	1.61	0.83
1:A:216:THR:HA	1:A:397:ALA:HB1	1.60	0.83
1:A:219:VAL:O	1:A:223:VAL:HG23	1.78	0.83
1:A:73:LEU:C	1:A:75:ILE:H	1.87	0.82
1:A:333:PHE:O	1:A:337:THR:HG22	1.78	0.82
1:A:356:ILE:HG22	1:A:358:GLY:H	1.45	0.82
1:A:393:ASN:HD21	1:A:402:THR:H	1.27	0.82
1:A:73:LEU:HD13	1:A:126:PHE:CE2	2.17	0.80
1:A:380:MET:HG2	2:B:18:CYS:HB3	1.65	0.79
1:A:68:GLY:HA2	1:A:73:LEU:H	1.49	0.78
1:A:124:VAL:HG22	1:A:144:ILE:HD13	1.64	0.78
1:A:183:PHE:CE1	2:B:49:ILE:HG13	2.18	0.77
1:A:360:ARG:HB3	1:A:365:ALA:HB1	1.65	0.77
1:A:52:ILE:HG12	1:A:132:PHE:HA	1.67	0.76
1:A:234:PRO:HB2	1:A:357:LYS:CB	2.15	0.76
1:A:356:ILE:HG22	1:A:357:LYS:N	2.00	0.76
3:C:36:VAL:O	3:C:39:ALA:HB3	1.86	0.76
1:A:231:VAL:HB	1:A:249:ILE:CG1	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HD12	1:A:52:ILE:O	1.86	0.74
1:A:358:GLY:O	1:A:359:PHE:HB2	1.86	0.74
1:A:380:MET:SD	2:B:22:TRP:HB2	2.28	0.74
1:A:374:ILE:HB	1:A:375:PRO:HD3	1.70	0.74
1:A:223:VAL:HG11	1:A:405:LEU:HA	1.69	0.73
1:A:76:GLY:O	1:A:78:ILE:N	2.21	0.73
1:A:183:PHE:HE1	2:B:49:ILE:HG13	1.52	0.73
1:A:273:GLY:CA	1:A:284:LEU:HD12	2.20	0.72
1:A:149:PHE:O	1:A:152:ILE:HB	1.89	0.72
1:A:3:LYS:HE3	1:A:3:LYS:HA	1.70	0.72
1:A:157:LEU:HD23	1:A:160:ILE:HD12	1.71	0.72
1:A:273:GLY:HA2	1:A:284:LEU:HD12	1.71	0.72
1:A:234:PRO:HB2	1:A:357:LYS:HB2	1.71	0.72
1:A:68:GLY:HA2	1:A:72:THR:HB	1.71	0.71
1:A:33:VAL:HG13	1:A:157:LEU:HD22	1.72	0.71
1:A:98:LEU:HA	1:A:103:ASN:HB2	1.71	0.71
1:A:251:PHE:CE1	1:A:381:SER:HA	2.26	0.71
1:A:229:MET:HE2	2:B:25:LEU:HD13	1.73	0.70
1:A:255:SER:C	1:A:258:PRO:HD2	2.16	0.70
1:A:328:VAL:O	1:A:332:ILE:HG13	1.92	0.69
1:A:82:GLY:HA2	1:A:111:GLN:NE2	2.07	0.69
1:A:393:ASN:HD21	1:A:402:THR:N	1.91	0.69
1:A:253:TYR:HE1	1:A:413:ARG:HH11	1.43	0.67
1:A:76:GLY:C	1:A:78:ILE:N	2.49	0.67
1:A:5:ILE:N	1:A:6:PRO:HD2	2.10	0.67
1:A:174:ILE:O	1:A:178:VAL:HG23	1.95	0.67
1:A:408:VAL:HG13	2:B:40:THR:HG21	1.77	0.67
1:A:103:ASN:HA	1:A:106:LEU:HD12	1.76	0.67
1:A:149:PHE:HB3	3:C:40:PHE:CZ	2.31	0.66
1:A:299:TYR:O	1:A:300:LEU:HD23	1.96	0.66
1:A:73:LEU:C	1:A:75:ILE:N	2.53	0.66
1:A:231:VAL:HB	1:A:249:ILE:HD11	1.77	0.66
3:C:32:HIS:O	3:C:36:VAL:HG23	1.96	0.65
1:A:281:ILE:N	1:A:281:ILE:HD12	2.11	0.65
1:A:164:TYR:CZ	3:C:30:PRO:HG2	2.31	0.65
1:A:76:GLY:C	1:A:78:ILE:H	2.04	0.65
1:A:388:LEU:O	1:A:391:ILE:HG22	1.96	0.64
1:A:82:GLY:HA2	1:A:111:GLN:HE21	1.62	0.64
1:A:102:GLU:O	1:A:106:LEU:HG	1.98	0.64
1:A:356:ILE:HG22	1:A:357:LYS:H	1.63	0.64
1:A:127:VAL:HG11	1:A:144:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:TYR:CD1	1:A:247:TYR:C	2.76	0.64
1:A:52:ILE:CG1	1:A:132:PHE:HA	2.28	0.63
1:A:164:TYR:CE1	3:C:30:PRO:HG2	2.34	0.63
1:A:82:GLY:O	1:A:86:GLN:HG2	1.97	0.63
1:A:257:ILE:HG21	1:A:334:TRP:CH2	2.33	0.63
1:A:189:PRO:HD3	2:B:56:VAL:HG22	1.81	0.63
1:A:342:PRO:O	1:A:343:LYS:C	2.41	0.63
1:A:157:LEU:O	1:A:161:VAL:HG23	1.99	0.63
1:A:240:ILE:HG22	1:A:241:LYS:N	2.09	0.62
1:A:355:ALA:HB2	1:A:361:LYS:HA	1.80	0.62
1:A:138:LEU:O	1:A:142:LEU:HG	1.99	0.62
1:A:228:CYS:SG	2:B:36:VAL:HG21	2.40	0.62
1:A:250:LYS:HD2	1:A:253:TYR:HD2	1.64	0.62
1:A:16:LEU:HD23	1:A:16:LEU:N	2.10	0.62
1:A:88:LEU:C	1:A:90:GLY:H	2.08	0.62
1:A:231:VAL:O	1:A:249:ILE:HG12	1.99	0.62
1:A:79:VAL:O	1:A:83:ILE:HG13	1.99	0.62
1:A:231:VAL:HB	1:A:249:ILE:HG13	1.80	0.62
1:A:231:VAL:HB	1:A:249:ILE:CD1	2.30	0.62
1:A:195:LYS:HB3	1:A:209:TYR:CD2	2.34	0.61
1:A:308:SER:HB3	1:A:394:PHE:O	2.00	0.61
1:A:14:VAL:HG21	1:A:159:GLU:HB3	1.81	0.61
1:A:98:LEU:HA	1:A:103:ASN:CB	2.30	0.61
1:A:156:TYR:O	1:A:160:ILE:HG13	2.00	0.61
1:A:235:LEU:HB2	1:A:245:GLY:HA3	1.83	0.61
1:A:152:ILE:HD13	1:A:155:ILE:HD12	1.82	0.61
1:A:188:GLY:HA2	2:B:52:TYR:HE1	1.65	0.61
1:A:379:VAL:CG1	2:B:18:CYS:SG	2.89	0.60
1:A:141:PHE:CZ	1:A:145:ILE:HD11	2.36	0.60
1:A:270:GLN:NE2	1:A:301:SER:HB3	2.17	0.60
1:A:254:VAL:HG13	1:A:381:SER:OG	2.02	0.60
1:A:123:ALA:HB2	1:A:148:ALA:HB2	1.84	0.60
1:A:85:MET:HE2	1:A:111:GLN:HB2	1.83	0.59
1:A:4:LEU:C	1:A:6:PRO:HD2	2.27	0.59
1:A:153:ILE:HD13	3:C:37:THR:HG23	1.84	0.59
1:A:340:LEU:HD12	1:A:340:LEU:N	2.14	0.59
1:A:250:LYS:NZ	1:A:416:GLU:OE1	2.32	0.59
1:A:287:TYR:CE2	1:A:292:ALA:HB2	2.37	0.59
1:A:374:ILE:CB	1:A:375:PRO:HD3	2.33	0.59
1:A:23:PHE:HD1	1:A:421:GLU:HB3	1.67	0.59
1:A:98:LEU:O	1:A:99:SER:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HD13	3:C:34:ILE:HD11	1.85	0.58
1:A:379:VAL:HG11	2:B:18:CYS:SG	2.43	0.58
1:A:247:TYR:C	1:A:247:TYR:HD1	2.09	0.58
1:A:281:ILE:HD12	1:A:281:ILE:H	1.67	0.58
1:A:216:THR:HA	1:A:397:ALA:CB	2.32	0.58
1:A:257:ILE:HG22	1:A:258:PRO:HD3	1.85	0.58
1:A:356:ILE:CG2	1:A:357:LYS:N	2.67	0.58
2:B:58:ALA:O	2:B:62:LYS:HG3	2.03	0.58
1:A:404:VAL:O	1:A:408:VAL:HG23	2.02	0.58
1:A:273:GLY:HA3	1:A:287:TYR:OH	2.03	0.58
1:A:13:GLU:HG3	1:A:14:VAL:N	2.15	0.58
2:B:49:ILE:O	2:B:53:ILE:HG13	2.04	0.58
1:A:86:GLN:O	1:A:333:PHE:HD2	1.87	0.58
1:A:116:ILE:HA	1:A:119:CYS:HB2	1.85	0.58
1:A:279:MET:O	1:A:279:MET:HG2	2.03	0.58
2:B:16:GLU:HA	2:B:16:GLU:OE2	2.04	0.58
1:A:379:VAL:HG11	2:B:14:PHE:HE1	1.69	0.57
1:A:250:LYS:O	1:A:254:VAL:HG12	2.04	0.57
1:A:328:VAL:HG13	1:A:379:VAL:HG22	1.87	0.57
1:A:68:GLY:CA	1:A:72:THR:HB	2.33	0.57
1:A:304:TYR:HD1	1:A:305:GLY:N	2.02	0.57
1:A:425:GLU:O	1:A:426:LEU:HD12	2.05	0.56
2:B:17:GLU:O	2:B:20:ARG:HB2	2.05	0.56
1:A:23:PHE:CD1	1:A:421:GLU:HB3	2.40	0.56
1:A:125:LEU:HD21	1:A:272:TRP:CD1	2.41	0.56
1:A:268:ASN:O	1:A:272:TRP:HB2	2.04	0.56
1:A:375:PRO:HB2	1:A:376:PRO:CD	2.36	0.56
1:A:70:LEU:O	1:A:71:ILE:HB	2.04	0.56
1:A:324:ILE:HD11	1:A:387:PHE:HB2	1.88	0.56
2:B:52:TYR:CE1	2:B:56:VAL:HG21	2.41	0.56
1:A:73:LEU:HD13	1:A:126:PHE:CD2	2.41	0.56
1:A:80:THR:HG23	1:A:268:ASN:ND2	2.20	0.56
1:A:355:ALA:HB3	1:A:361:LYS:HG2	1.88	0.56
1:A:15:GLU:OE1	1:A:17:PRO:HG3	2.04	0.56
1:A:325:ILE:HG13	1:A:326:THR:N	2.20	0.56
1:A:321:ILE:O	1:A:325:ILE:HG23	2.06	0.55
1:A:55:ILE:O	1:A:69:THR:HB	2.06	0.55
1:A:306:LEU:N	1:A:306:LEU:HD12	2.22	0.55
2:B:4:PHE:O	2:B:8:ILE:HG13	2.07	0.55
1:A:89:VAL:HG21	1:A:107:PHE:CD1	2.41	0.55
1:A:345:MET:O	1:A:349:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ILE:N	1:A:116:ILE:HD12	2.22	0.55
1:A:85:MET:HB3	1:A:107:PHE:CE1	2.42	0.55
1:A:91:SER:OG	1:A:93:ILE:HG13	2.06	0.55
1:A:76:GLY:O	1:A:77:PRO:C	2.49	0.55
1:A:102:GLU:C	1:A:106:LEU:HG	2.32	0.54
1:A:317:ILE:O	1:A:321:ILE:HG13	2.08	0.54
3:C:22:THR:HG22	3:C:24:SER:H	1.72	0.54
1:A:257:ILE:HG21	1:A:334:TRP:CZ2	2.42	0.54
2:B:66:LYS:HB2	2:B:66:LYS:NZ	2.22	0.54
2:B:55:HIS:O	2:B:56:VAL:C	2.50	0.54
1:A:29:TRP:NE1	1:A:164:TYR:HD2	2.05	0.54
1:A:211:ALA:HB3	1:A:212:PRO:CD	2.38	0.54
1:A:274:LEU:O	1:A:277:TYR:HB3	2.08	0.54
1:A:340:LEU:H	1:A:340:LEU:CD1	2.14	0.54
1:A:356:ILE:CG2	1:A:357:LYS:H	2.21	0.53
1:A:225:TYR:C	1:A:225:TYR:CD2	2.85	0.53
1:A:342:PRO:HA	1:A:345:MET:HB2	1.90	0.53
1:A:148:ALA:O	1:A:152:ILE:HG12	2.08	0.53
1:A:182:ILE:HA	1:A:398:LEU:HD23	1.89	0.53
1:A:240:ILE:C	1:A:241:LYS:HG3	2.32	0.53
1:A:255:SER:HA	1:A:258:PRO:HG2	1.90	0.53
1:A:260:ILE:O	1:A:264:ALA:HB2	2.07	0.53
1:A:355:ALA:CB	1:A:361:LYS:HG2	2.39	0.53
2:B:16:GLU:O	2:B:19:ARG:HB2	2.08	0.53
1:A:188:GLY:HA2	2:B:52:TYR:CE1	2.43	0.53
1:A:85:MET:HG3	1:A:111:GLN:HG3	1.90	0.53
2:B:36:VAL:O	2:B:37:ALA:C	2.52	0.53
1:A:72:THR:O	1:A:75:ILE:HB	2.09	0.52
1:A:256:ASN:HD21	1:A:409:SER:CB	2.21	0.52
1:A:259:VAL:CG1	1:A:406:LEU:HD21	2.38	0.52
1:A:15:GLU:O	1:A:17:PRO:HD3	2.09	0.52
1:A:166:ILE:HD13	1:A:418:LEU:CD2	2.39	0.52
1:A:379:VAL:HG12	1:A:380:MET:N	2.25	0.52
1:A:379:VAL:HG12	2:B:18:CYS:SG	2.50	0.52
1:A:146:GLN:HG2	3:C:44:GLU:OE1	2.10	0.52
2:B:32:GLU:O	2:B:35:ALA:HB3	2.09	0.52
1:A:312:ASP:N	1:A:313:PRO:HD3	2.25	0.52
3:C:34:ILE:O	3:C:38:VAL:HG23	2.10	0.52
1:A:22:THR:HG1	1:A:25:GLU:HG3	1.75	0.52
1:A:274:LEU:C	1:A:274:LEU:HD13	2.34	0.52
1:A:257:ILE:HG22	1:A:258:PRO:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:HG23	1:A:268:ASN:HD21	1.74	0.52
1:A:94:ILE:O	1:A:94:ILE:HG22	2.10	0.52
1:A:250:LYS:CD	1:A:253:TYR:HD2	2.22	0.52
2:B:62:LYS:O	2:B:66:LYS:HB2	2.09	0.52
1:A:257:ILE:N	1:A:258:PRO:CD	2.72	0.51
1:A:160:ILE:HD11	3:C:33:VAL:CG2	2.41	0.51
1:A:260:ILE:HG12	1:A:406:LEU:HD13	1.91	0.51
1:A:337:THR:O	1:A:338:THR:C	2.51	0.51
1:A:135:LEU:H	1:A:135:LEU:HD12	1.75	0.51
1:A:320:MET:O	1:A:324:ILE:HG12	2.11	0.51
1:A:343:LYS:O	1:A:346:ALA:HB3	2.10	0.51
1:A:118:MET:HE3	1:A:122:GLU:HG2	1.92	0.51
1:A:160:ILE:HD13	3:C:34:ILE:CD1	2.41	0.51
1:A:425:GLU:O	1:A:425:GLU:HG3	2.10	0.51
1:A:256:ASN:HD21	1:A:409:SER:HB2	1.76	0.51
1:A:84:ILE:CD1	1:A:114:LEU:HD21	2.27	0.51
1:A:93:ILE:HG22	1:A:94:ILE:HG13	1.92	0.51
1:A:362:SER:HB2	1:A:365:ALA:CB	2.41	0.51
1:A:90:GLY:C	1:A:92:GLY:H	2.18	0.50
1:A:332:ILE:O	1:A:335:VAL:HB	2.12	0.50
1:A:80:THR:O	1:A:83:ILE:HB	2.11	0.50
1:A:71:ILE:HG22	1:A:71:ILE:O	2.10	0.50
1:A:260:ILE:HG12	1:A:406:LEU:CD1	2.42	0.50
1:A:362:SER:HB2	1:A:365:ALA:HB2	1.94	0.50
1:A:86:GLN:O	1:A:90:GLY:HA3	2.11	0.50
1:A:179:SER:OG	2:B:44:ILE:HG23	2.12	0.50
1:A:250:LYS:HB3	1:A:253:TYR:HB3	1.92	0.50
1:A:70:LEU:O	1:A:71:ILE:CB	2.60	0.50
1:A:87:LEU:HD21	1:A:329:MET:HE1	1.94	0.50
2:B:21:VAL:C	2:B:23:LEU:H	2.18	0.50
1:A:274:LEU:HD23	1:A:287:TYR:CD2	2.47	0.50
2:B:49:ILE:O	2:B:52:TYR:HB3	2.12	0.50
1:A:89:VAL:HG21	1:A:107:PHE:HD1	1.77	0.49
1:A:304:TYR:CD1	1:A:304:TYR:C	2.89	0.49
1:A:340:LEU:O	1:A:342:PRO:HD3	2.12	0.49
2:B:29:THR:O	2:B:32:GLU:HB3	2.12	0.49
1:A:374:ILE:CB	1:A:375:PRO:CD	2.89	0.49
1:A:252:VAL:HG23	1:A:253:TYR:H	1.77	0.49
1:A:3:LYS:C	1:A:5:ILE:H	2.19	0.49
1:A:35:VAL:HG13	2:B:54:ILE:HD11	1.95	0.49
1:A:189:PRO:C	1:A:191:GLY:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:HD13	1:A:155:ILE:CD1	2.41	0.49
1:A:374:ILE:HB	1:A:375:PRO:CD	2.40	0.49
1:A:8:LEU:HD21	3:C:23:PHE:HB2	1.94	0.49
1:A:423:VAL:C	1:A:425:GLU:N	2.71	0.49
1:A:206:ASN:OD1	1:A:208:GLU:HB2	2.13	0.49
1:A:362:SER:O	1:A:365:ALA:HB3	2.13	0.49
1:A:21:ILE:HD12	1:A:21:ILE:H	1.78	0.49
1:A:100:ILE:HG22	1:A:102:GLU:H	1.76	0.49
1:A:51:GLN:CD	1:A:51:GLN:H	2.20	0.49
1:A:84:ILE:O	1:A:87:LEU:HB2	2.13	0.49
1:A:142:LEU:O	1:A:145:ILE:HB	2.12	0.49
1:A:187:LEU:CD2	1:A:193:LEU:HD23	2.42	0.48
1:A:204:VAL:O	1:A:204:VAL:HG23	2.12	0.48
1:A:252:VAL:HG23	1:A:253:TYR:N	2.28	0.48
1:A:287:TYR:HB3	1:A:291:ARG:O	2.13	0.48
1:A:293:VAL:O	1:A:293:VAL:HG12	2.13	0.48
1:A:293:VAL:O	1:A:294:ASP:HB2	2.13	0.48
3:C:30:PRO:O	3:C:33:VAL:HG23	2.14	0.48
1:A:216:THR:CA	1:A:397:ALA:HB1	2.39	0.48
1:A:374:ILE:O	1:A:375:PRO:C	2.56	0.48
2:B:8:ILE:O	2:B:12:LYS:HG3	2.12	0.48
1:A:21:ILE:HD13	1:A:26:LYS:HE3	1.94	0.48
1:A:169:GLY:O	1:A:170:ILE:C	2.54	0.48
1:A:410:ILE:HA	1:A:413:ARG:HG2	1.95	0.48
1:A:304:TYR:CD1	1:A:305:GLY:N	2.82	0.48
1:A:314:ILE:HD12	1:A:315:HIS:N	2.18	0.48
1:A:374:ILE:HG22	1:A:375:PRO:N	2.29	0.48
1:A:405:LEU:O	1:A:406:LEU:C	2.55	0.48
1:A:34:LEU:O	1:A:37:TYR:HB3	2.14	0.48
1:A:229:MET:CE	2:B:25:LEU:HD13	2.43	0.48
1:A:314:ILE:CD1	1:A:315:HIS:H	2.19	0.48
1:A:370:LEU:C	1:A:372:ARG:N	2.70	0.48
1:A:384:PHE:O	1:A:385:VAL:C	2.56	0.47
2:B:53:ILE:O	2:B:57:PRO:HG3	2.14	0.47
1:A:73:LEU:O	1:A:75:ILE:N	2.47	0.47
1:A:225:TYR:C	1:A:225:TYR:HD2	2.22	0.47
3:C:31:GLU:H	3:C:31:GLU:CD	2.20	0.47
1:A:274:LEU:O	1:A:274:LEU:HD13	2.14	0.47
1:A:151:SER:O	1:A:155:ILE:HG13	2.13	0.47
1:A:223:VAL:CG1	1:A:405:LEU:HA	2.40	0.47
1:A:276:LEU:HD23	1:A:279:MET:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PHE:O	1:A:360:ARG:HB2	2.14	0.47
1:A:8:LEU:HD23	1:A:8:LEU:C	2.39	0.47
1:A:23:PHE:CE2	1:A:27:LEU:HD12	2.50	0.47
1:A:129:ALA:O	1:A:278:ARG:HD3	2.15	0.47
1:A:423:VAL:C	1:A:425:GLU:H	2.22	0.47
1:A:149:PHE:HB3	3:C:40:PHE:HZ	1.77	0.47
1:A:238:GLY:O	1:A:239:ARG:HB2	2.15	0.47
1:A:370:LEU:C	1:A:372:ARG:H	2.22	0.47
1:A:94:ILE:O	1:A:96:MET:HG3	2.14	0.47
1:A:149:PHE:HD2	3:C:40:PHE:HZ	1.63	0.47
1:A:73:LEU:HD13	1:A:126:PHE:CZ	2.50	0.47
1:A:407:THR:O	1:A:411:VAL:HG23	2.15	0.47
2:B:13:GLU:O	2:B:16:GLU:HB3	2.16	0.46
2:B:14:PHE:CD1	2:B:14:PHE:C	2.94	0.46
1:A:69:THR:O	1:A:70:LEU:HG	2.15	0.46
1:A:83:ILE:HG23	1:A:330:PHE:CZ	2.51	0.46
1:A:112:LYS:O	1:A:115:SER:HB3	2.15	0.46
1:A:253:TYR:HD1	1:A:256:ASN:HD22	1.64	0.46
1:A:52:ILE:CD1	1:A:132:PHE:HA	2.45	0.46
1:A:2:LYS:O	1:A:3:LYS:HG2	2.16	0.46
1:A:5:ILE:N	1:A:6:PRO:CD	2.78	0.46
1:A:98:LEU:O	1:A:100:ILE:N	2.49	0.46
1:A:108:GLN:O	1:A:109:GLY:C	2.59	0.46
1:A:14:VAL:CG2	1:A:159:GLU:HB3	2.45	0.46
1:A:13:GLU:CG	1:A:14:VAL:H	2.23	0.46
1:A:35:VAL:O	1:A:39:ILE:HG12	2.16	0.46
1:A:206:ASN:HB3	1:A:209:TYR:HD1	1.81	0.46
1:A:46:TYR:HB3	1:A:146:GLN:NE2	2.21	0.46
1:A:256:ASN:N	1:A:258:PRO:HD2	2.31	0.45
1:A:328:VAL:HG12	1:A:332:ILE:HD11	1.98	0.45
1:A:381:SER:O	1:A:384:PHE:HB3	2.16	0.45
1:A:391:ILE:O	1:A:395:ILE:HG22	2.16	0.45
2:B:64:ILE:O	2:B:65:LEU:HD23	2.16	0.45
1:A:91:SER:C	1:A:93:ILE:H	2.23	0.45
1:A:338:THR:HG22	1:A:339:GLY:N	2.31	0.45
1:A:22:THR:OG1	1:A:25:GLU:HG3	2.15	0.45
1:A:88:LEU:C	1:A:90:GLY:N	2.65	0.45
1:A:195:LYS:HD3	1:A:209:TYR:HE2	1.82	0.45
1:A:310:ILE:C	1:A:312:ASP:H	2.23	0.45
1:A:76:GLY:O	1:A:79:VAL:N	2.50	0.45
1:A:194:TRP:HA	1:A:194:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:PRO:HG3	1:A:374:ILE:HD11	1.99	0.45
1:A:46:TYR:CB	1:A:146:GLN:HE22	2.22	0.45
1:A:92:GLY:O	1:A:95:GLN:HG3	2.16	0.45
3:C:44:GLU:HA	3:C:47:LEU:HB3	1.99	0.45
1:A:98:LEU:O	1:A:100:ILE:O	2.35	0.45
2:B:35:ALA:HA	2:B:38:LYS:HE3	1.99	0.45
1:A:77:PRO:HG3	1:A:119:CYS:HA	1.98	0.44
1:A:211:ALA:HA	1:A:214:ILE:HD12	1.99	0.44
1:A:281:ILE:N	1:A:281:ILE:CD1	2.80	0.44
3:C:30:PRO:O	3:C:34:ILE:HG12	2.18	0.44
1:A:74:GLY:O	1:A:76:GLY:N	2.50	0.44
1:A:195:LYS:HD3	1:A:209:TYR:CE2	2.52	0.44
2:B:24:VAL:HG12	2:B:24:VAL:O	2.17	0.44
1:A:166:ILE:HG22	1:A:167:GLY:H	1.83	0.44
1:A:265:LEU:O	1:A:269:ILE:HG13	2.18	0.44
1:A:34:LEU:HD11	1:A:38:PHE:CZ	2.52	0.44
1:A:42:CYS:SG	2:B:55:HIS:HA	2.58	0.44
2:B:29:THR:O	2:B:32:GLU:N	2.51	0.44
3:C:39:ALA:O	3:C:40:PHE:C	2.60	0.44
1:A:86:GLN:NE2	1:A:107:PHE:HZ	2.15	0.44
1:A:234:PRO:CB	1:A:357:LYS:HB2	2.46	0.44
1:A:89:VAL:HG12	1:A:89:VAL:O	2.17	0.44
1:A:188:GLY:CA	2:B:52:TYR:HE1	2.30	0.44
1:A:259:VAL:HG12	1:A:406:LEU:HD21	2.00	0.44
1:A:113:LEU:C	1:A:113:LEU:HD13	2.42	0.44
1:A:240:ILE:O	1:A:241:LYS:HG3	2.18	0.44
1:A:405:LEU:C	1:A:405:LEU:HD23	2.43	0.44
1:A:14:VAL:CG1	3:C:30:PRO:HG3	2.48	0.44
1:A:16:LEU:H	1:A:16:LEU:CD2	2.11	0.44
1:A:149:PHE:HB3	3:C:40:PHE:CE2	2.52	0.44
1:A:376:PRO:HB3	2:B:17:GLU:HB3	2.00	0.44
1:A:14:VAL:HA	3:C:28:VAL:O	2.17	0.43
1:A:187:LEU:HD21	1:A:193:LEU:CD2	2.48	0.43
1:A:417:GLN:HE21	1:A:417:GLN:HB2	1.52	0.43
1:A:88:LEU:O	1:A:90:GLY:N	2.50	0.43
1:A:135:LEU:HD12	1:A:135:LEU:N	2.33	0.43
1:A:187:LEU:HD21	1:A:193:LEU:HD23	2.01	0.43
1:A:145:ILE:O	1:A:146:GLN:C	2.60	0.43
1:A:270:GLN:HE22	1:A:301:SER:HB3	1.82	0.43
3:C:49:TYR:CD1	3:C:49:TYR:N	2.85	0.43
1:A:197:LEU:O	1:A:200:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PHE:O	1:A:360:ARG:CB	2.66	0.43
1:A:350:GLY:O	1:A:353:GLY:N	2.51	0.43
1:A:360:ARG:O	1:A:366:ILE:HG13	2.19	0.43
1:A:153:ILE:HD11	3:C:40:PHE:CD1	2.53	0.43
1:A:80:THR:HG21	1:A:118:MET:HE2	2.01	0.43
1:A:14:VAL:HG21	1:A:159:GLU:CB	2.48	0.43
1:A:35:VAL:O	1:A:36:LEU:C	2.62	0.43
1:A:71:ILE:O	1:A:71:ILE:CG2	2.67	0.43
1:A:166:ILE:HG22	1:A:167:GLY:N	2.34	0.43
1:A:194:TRP:HA	1:A:194:TRP:HE3	1.84	0.43
1:A:231:VAL:CB	1:A:249:ILE:HD11	2.48	0.43
1:A:247:TYR:CD1	1:A:248:PRO:N	2.87	0.43
1:A:314:ILE:O	1:A:318:VAL:HG23	2.18	0.43
1:A:331:GLY:O	1:A:334:TRP:HB3	2.18	0.43
1:A:118:MET:O	1:A:122:GLU:HG2	2.19	0.43
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.82	0.43
1:A:341:ASP:O	1:A:341:ASP:OD1	2.37	0.43
1:A:5:ILE:O	1:A:9:GLU:HG3	2.19	0.42
1:A:322:ALA:O	1:A:325:ILE:HG12	2.19	0.42
1:A:400:GLY:O	1:A:401:GLY:C	2.61	0.42
2:B:66:LYS:O	2:B:66:LYS:HG2	2.17	0.42
1:A:75:ILE:HD13	1:A:122:GLU:OE2	2.19	0.42
3:C:30:PRO:HA	3:C:33:VAL:CG2	2.49	0.42
1:A:384:PHE:O	1:A:387:PHE:HB3	2.19	0.42
2:B:30:LYS:HD3	2:B:30:LYS:HA	1.91	0.42
1:A:251:PHE:C	1:A:254:VAL:HG12	2.44	0.42
1:A:13:GLU:O	3:C:28:VAL:HB	2.19	0.42
1:A:51:GLN:OE1	1:A:51:GLN:N	2.52	0.42
1:A:83:ILE:HG12	1:A:261:LEU:HD22	2.01	0.42
2:B:34:LEU:O	2:B:38:LYS:HG3	2.19	0.42
1:A:26:LYS:HA	1:A:164:TYR:O	2.20	0.42
1:A:85:MET:HG3	1:A:111:GLN:CG	2.49	0.42
1:A:310:ILE:O	1:A:312:ASP:N	2.44	0.42
1:A:55:ILE:O	1:A:69:THR:CB	2.68	0.42
1:A:202:GLN:OE1	1:A:202:GLN:HA	2.20	0.42
1:A:316:ALA:O	1:A:317:ILE:C	2.61	0.42
1:A:317:ILE:HD12	1:A:317:ILE:H	1.85	0.42
1:A:410:ILE:O	1:A:414:MET:HB2	2.20	0.42
2:B:56:VAL:HB	2:B:57:PRO:CD	2.50	0.42
1:A:166:ILE:HD13	1:A:418:LEU:HD21	2.01	0.42
2:B:35:ALA:O	2:B:38:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLY:HA3	1:A:278:ARG:NH1	2.34	0.41
1:A:382:SER:O	1:A:383:ALA:C	2.63	0.41
2:B:21:VAL:C	2:B:23:LEU:N	2.78	0.41
1:A:274:LEU:N	1:A:287:TYR:CZ	2.89	0.41
1:A:296:ILE:O	1:A:297:ALA:C	2.63	0.41
1:A:219:VAL:HG12	1:A:220:PHE:N	2.36	0.41
1:A:18:VAL:HG12	1:A:18:VAL:O	2.20	0.41
1:A:5:ILE:HA	1:A:8:LEU:HB3	2.02	0.41
1:A:157:LEU:HA	1:A:160:ILE:HD12	2.03	0.41
1:A:6:PRO:HG2	1:A:7:ILE:H	1.86	0.41
1:A:313:PRO:O	1:A:317:ILE:HD13	2.21	0.41
3:C:30:PRO:O	3:C:31:GLU:C	2.63	0.41
3:C:31:GLU:OE2	3:C:31:GLU:N	2.37	0.41
1:A:136:THR:O	1:A:137:PRO:C	2.64	0.41
1:A:375:PRO:HB2	1:A:376:PRO:HD3	2.02	0.41
2:B:16:GLU:O	2:B:20:ARG:HD3	2.20	0.41
1:A:52:ILE:HD11	1:A:132:PHE:HA	2.03	0.41
1:A:147:ILE:HG22	1:A:148:ALA:N	2.35	0.41
1:A:183:PHE:CZ	2:B:45:SER:HA	2.56	0.41
1:A:224:VAL:HG12	2:B:33:TYR:CE1	2.56	0.41
2:B:14:PHE:CE1	2:B:18:CYS:SG	3.14	0.41
1:A:156:TYR:HB3	3:C:33:VAL:HG11	2.03	0.41
1:A:342:PRO:HG3	1:A:374:ILE:CD1	2.51	0.41
1:A:393:ASN:ND2	1:A:402:THR:H	2.07	0.41
1:A:143:VAL:O	1:A:144:ILE:C	2.63	0.40
1:A:235:LEU:HB3	1:A:354:MET:HE2	2.02	0.40
1:A:419:LEU:C	1:A:421:GLU:N	2.79	0.40
2:B:9:GLU:O	2:B:12:LYS:HB2	2.21	0.40
1:A:181:THR:HG21	1:A:399:GLY:HA2	2.04	0.40
1:A:218:ILE:O	1:A:219:VAL:C	2.63	0.40
1:A:295:GLY:O	1:A:296:ILE:C	2.63	0.40
3:C:37:THR:C	3:C:39:ALA:N	2.77	0.40
3:C:50:GLY:O	3:C:51:ARG:C	2.64	0.40
1:A:216:THR:O	1:A:217:ILE:C	2.63	0.40
1:A:302:THR:HA	1:A:303:PRO:HD3	1.83	0.40
1:A:198:ASN:OD1	1:A:198:ASN:C	2.64	0.40
1:A:230:ARG:HD3	1:A:248:PRO:HB2	2.04	0.40
1:A:333:PHE:N	1:A:333:PHE:CD1	2.89	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	420/426 (99%)	290 (69%)	86 (20%)	44 (10%)	0	5
2	B	63/74 (85%)	51 (81%)	7 (11%)	5 (8%)	1	8
3	C	30/53 (57%)	22 (73%)	6 (20%)	2 (7%)	1	11
All	All	513/553 (93%)	363 (71%)	99 (19%)	51 (10%)	0	6

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	PRO
1	A	71	ILE
1	A	72	THR
1	A	75	ILE
1	A	99	SER
1	A	246	LYS
1	A	338	THR
1	A	360	ARG
1	A	70	LEU
1	A	145	ILE
1	A	147	ILE
1	A	188	GLY
1	A	189	PRO
1	A	237	HIS
1	A	245	GLY
1	A	311	SER
1	A	339	GLY
1	A	359	PHE
1	A	385	VAL
1	A	396	GLY
2	B	55	HIS
1	A	363	GLU
1	A	4	LEU
1	A	19	LYS

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Mol	Chain	Res	Type
1	A	67	GLY
1	A	77	PRO
1	A	102	GLU
1	A	240	ILE
1	A	346	ALA
1	A	367	GLU
1	A	374	ILE
1	A	429	ALA
1	A	430	ILE
2	B	38	LYS
1	A	172	LEU
1	A	205	PRO
1	A	244	VAL
1	A	288	GLU
1	A	356	ILE
2	B	30	LYS
3	C	51	ARG
1	A	6	PRO
3	C	41	VAL
2	B	24	VAL
2	B	56	VAL
1	A	89	VAL
1	A	137	PRO
1	A	211	ALA
1	A	375	PRO
1	A	170	ILE
1	A	248	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	341/345 (99%)	310 (91%)	31 (9%)	9	33
2	B	57/66 (86%)	53 (93%)	4 (7%)	14	41
3	C	28/45 (62%)	26 (93%)	2 (7%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	426/456 (93%)	389 (91%)	37 (9%)	9 34

All (37) 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	27	LEU
1	A	33	VAL
1	A	51	GLN
1	A	55	ILE
1	A	78	ILE
1	A	126	PHE
1	A	172	LEU
1	A	197	LEU
1	A	202	GLN
1	A	213	ILE
1	A	219	VAL
1	A	247	TYR
1	A	248	PRO
1	A	254	VAL
1	A	257	ILE
1	A	259	VAL
1	A	281	ILE
1	A	306	LEU
1	A	314	ILE
1	A	336	GLU
1	A	340	LEU
1	A	344	SER
1	A	363	GLU
1	A	375	PRO
1	A	379	VAL
1	A	380	MET
1	A	402	THR
1	A	417	GLN
2	B	19	ARG
2	B	30	LYS
2	B	42	LEU
2	B	66	LYS
3	C	33	VAL
3	C	44	GLU

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	315	HIS
1	A	393	ASN
1	A	417	GLN
2	B	5	ASN
2	B	6	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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/426 (99%)	0.88	72 (17%) 4 4	48, 116, 167, 198	0
2	B	65/74 (87%)	0.25	2 (3%) 51 29	53, 120, 165, 180	0
3	C	32/53 (60%)	0.62	2 (6%) 26 16	111, 144, 176, 188	0
All	All	519/553 (93%)	0.79	76 (14%) 6 6	48, 119, 170, 198	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	THR	9.6
1	A	126	PHE	6.3
1	A	73	LEU	5.6
1	A	45	VAL	5.6
1	A	398	LEU	5.4
1	A	131	ALA	5.2
1	A	132	PHE	5.1
1	A	340	LEU	4.7
1	A	71	ILE	4.7
1	A	293	VAL	4.6
1	A	422	LYS	4.5
1	A	129	ALA	4.4
2	B	24	VAL	4.2
1	A	75	ILE	4.2
1	A	74	GLY	4.1
1	A	433	LEU	4.0
1	A	12	PRO	3.9
1	A	41	GLY	3.8
1	A	309	VAL	3.8
1	A	21	ILE	3.7
1	A	54	ALA	3.6
1	A	354	MET	3.6
1	A	427	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	417	GLN	3.5
1	A	55	ILE	3.4
1	A	305	GLY	3.2
1	A	306	LEU	3.2
1	A	246	LYS	3.2
1	A	413	ARG	3.2
1	A	241	LYS	3.1
1	A	339	GLY	3.1
1	A	14	VAL	3.0
1	A	95	GLN	3.0
1	A	72	THR	3.0
1	A	77	PRO	3.0
1	A	149	PHE	3.0
1	A	49	GLY	2.8
3	C	28	VAL	2.7
1	A	48	ALA	2.6
1	A	304	TYR	2.6
1	A	11	ILE	2.6
1	A	31	GLY	2.6
3	C	51	ARG	2.6
1	A	240	ILE	2.5
2	B	23	LEU	2.5
1	A	237	HIS	2.5
1	A	347	LYS	2.5
1	A	127	VAL	2.5
1	A	359	PHE	2.5
1	A	234	PRO	2.5
1	A	399	GLY	2.5
1	A	361	LYS	2.4
1	A	332	ILE	2.4
1	A	245	GLY	2.4
1	A	284	LEU	2.4
1	A	352	LEU	2.4
1	A	51	GLN	2.3
1	A	303	PRO	2.3
1	A	290	GLY	2.3
1	A	349	ILE	2.3
1	A	98	LEU	2.3
1	A	430	ILE	2.2
1	A	128	GLY	2.2
1	A	136	THR	2.2
1	A	229	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	4	LEU	2.2
1	A	56	PHE	2.2
1	A	139	LEU	2.2
1	A	10	LYS	2.1
1	A	20	GLU	2.1
1	A	233	ILE	2.1
1	A	351	SER	2.1
1	A	134	ILE	2.1
1	A	252	VAL	2.1
1	A	69	THR	2.1
1	A	130	GLY	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 oligosaccharides 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.