



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:58 PM GMT

PDB ID : 1RHZ
Title : The structure of a protein conducting channel
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Deposited on : 2003-11-15
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

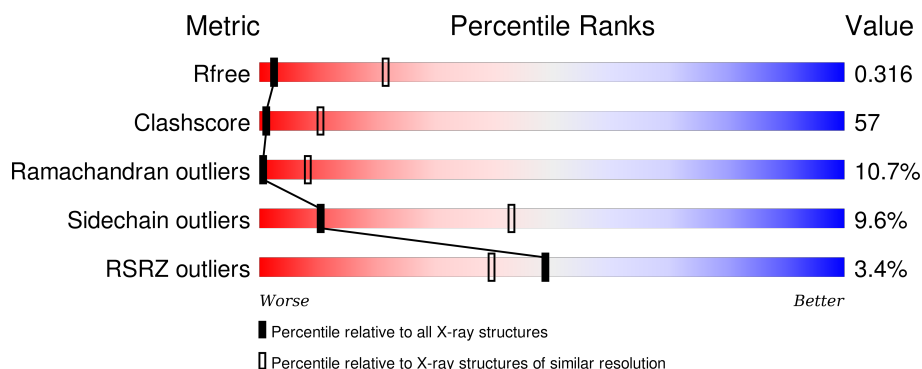
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

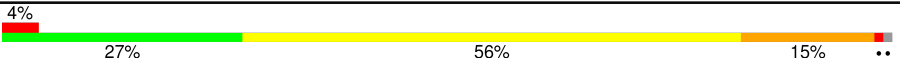
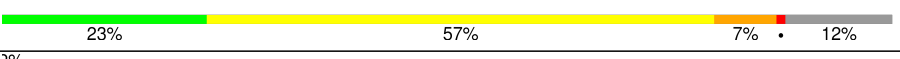

The reported resolution of this entry is 3.50 Å.

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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	436	 4% 27% 56% 15% ..
2	B	74	 23% 57% 7% • 12%
3	C	53	 2% 25% 34% • 40%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4090 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 secY subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3309	2210	521	559	19			

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

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

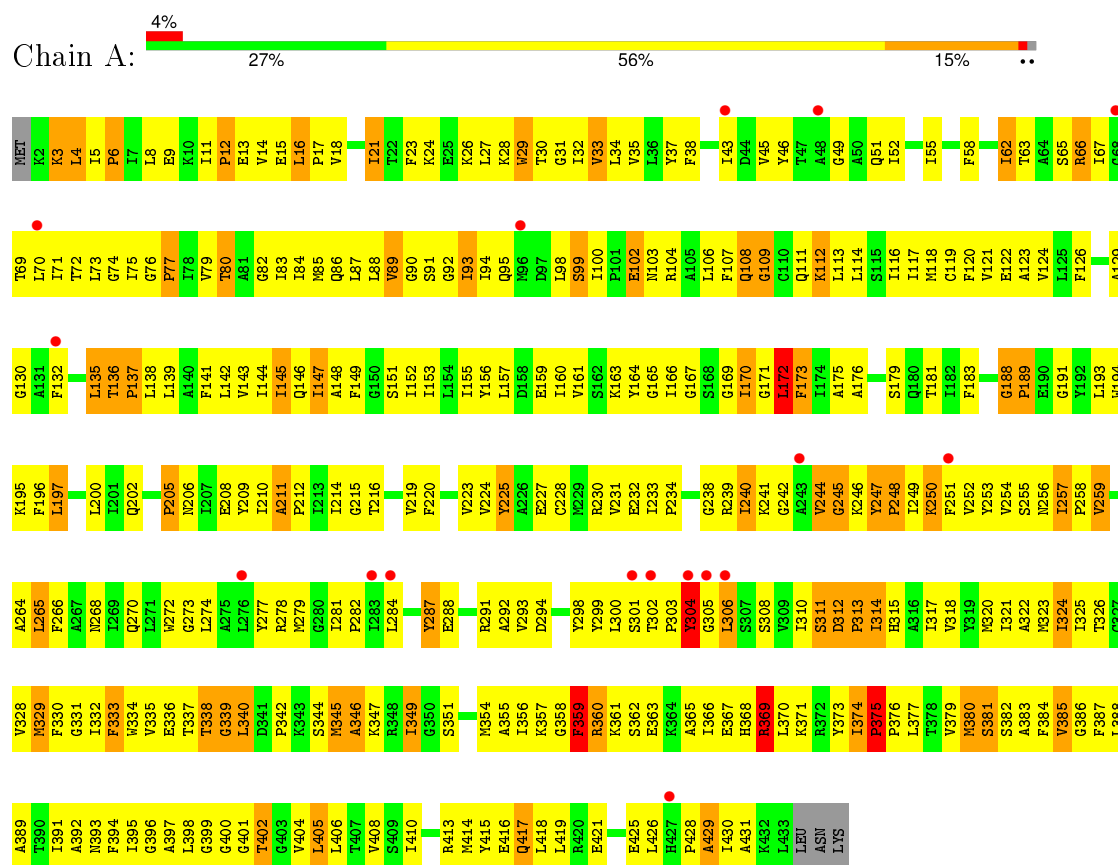
- Molecule 3 is a protein called SecBeta.

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

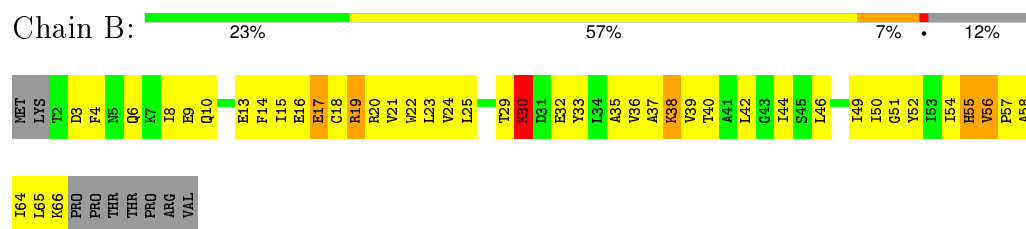
3 Residue-property plots

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.

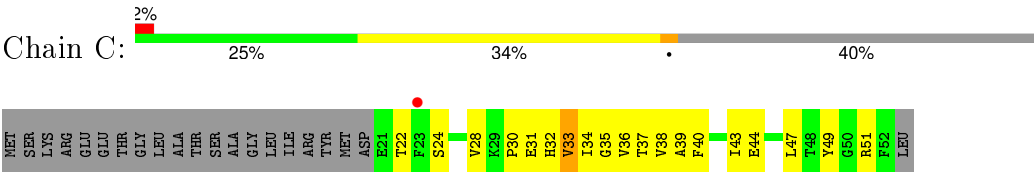
• Molecule 1: Preprotein translocase secY subunit



• Molecule 2: Preprotein translocase secE subunit



• Molecule 3: SecBeta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.75Å 149.36Å 79.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 3.50 58.17 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.6 (9.99-3.50) 97.9 (58.17-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.254 , 0.330 0.256 , 0.316	Depositor DCC
R_{free} test set	669 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 122.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 16798 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4090	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.44	0/3383	0.65	0/4593
2	B	0.43	0/533	0.62	0/719
3	C	0.38	0/262	0.55	0/354
All	All	0.43	0/4178	0.64	0/5666

There are no bond length outliers.

There are no bond angle outliers.

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	3309	0	3523	429	0
2	B	524	0	567	61	0
3	C	257	0	272	31	0
All	All	4090	0	4362	484	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 57.

All (484) 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	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD12	1:A:62:ILE:H	1.10	1.12
1:A:240:ILE:HG22	1:A:241:LYS:H	1.18	1.03
1:A:16:LEU:HD23	1:A:16:LEU:H	1.24	1.02
1:A:189:PRO:HD3	2:B:56:VAL:HG22	1.45	0.99
1:A:11:ILE:HD11	1:A:113:LEU:HD23	1.44	0.99
1:A:287:TYR:HA	1:A:292:ALA:HA	1.46	0.97
1:A:426:LEU:O	1:A:428:PRO:HD3	1.67	0.94
1:A:67:ILE:HA	1:A:72:THR:HG23	1.49	0.94
1:A:98:LEU:HA	1:A:103:ASN:HB2	1.46	0.93
1:A:124:VAL:HG22	1:A:144:ILE:HD13	1.51	0.93
1:A:73:LEU:HD21	1:A:122:GLU:HB2	1.53	0.91
1:A:13:GLU:HG3	1:A:14:VAL:H	1.36	0.90
1:A:157:LEU:HD23	1:A:160:ILE:HD12	1.53	0.90
1:A:46:TYR:HB3	1:A:146:GLN:HE22	1.38	0.89
1:A:80:THR:HG23	1:A:268:ASN:ND2	1.88	0.88
1:A:82:GLY:HA2	1:A:111:GLN:NE2	1.88	0.88
1:A:195:LYS:HB3	1:A:209:TYR:CD2	2.09	0.88
1:A:62:ILE:H	1:A:62:ILE:CD1	1.87	0.87
1:A:82:GLY:HA2	1:A:111:GLN:HE21	1.38	0.86
3:C:44:GLU:HA	3:C:47:LEU:HB3	1.58	0.84
1:A:223:VAL:HG11	1:A:405:LEU:HA	1.56	0.83
1:A:333:PHE:O	1:A:337:THR:HG22	1.79	0.83
1:A:250:LYS:HD2	1:A:253:TYR:HD2	1.43	0.83
1:A:153:ILE:HD13	3:C:37:THR:HG23	1.59	0.83
1:A:314:ILE:HD12	1:A:315:HIS:H	1.42	0.83
1:A:29:TRP:O	1:A:32:ILE:HG22	1.79	0.82
1:A:340:LEU:H	1:A:340:LEU:HD12	1.46	0.81
1:A:227:GLU:HA	1:A:252:VAL:HG21	1.61	0.81
1:A:63:THR:HG23	1:A:76:GLY:H	1.46	0.81
1:A:408:VAL:HG13	2:B:40:THR:HG21	1.62	0.80
1:A:195:LYS:HD3	1:A:209:TYR:HE2	1.46	0.79
1:A:328:VAL:HG12	1:A:332:ILE:HD11	1.64	0.79
1:A:33:VAL:HG21	1:A:161:VAL:HG22	1.63	0.79
1:A:98:LEU:HA	1:A:103:ASN:CB	2.13	0.78
1:A:374:ILE:HB	1:A:375:PRO:HD3	1.66	0.78
1:A:328:VAL:O	1:A:332:ILE:HG13	1.84	0.77
1:A:157:LEU:O	1:A:161:VAL:HG23	1.84	0.77
1:A:230:ARG:HD3	1:A:248:PRO:HB2	1.65	0.77
1:A:244:VAL:HG12	1:A:245:GLY:N	2.00	0.77
1:A:240:ILE:HG22	1:A:241:LYS:N	1.97	0.76
1:A:393:ASN:HD21	1:A:402:THR:H	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ALA:O	2:B:62:LYS:HG3	1.86	0.75
1:A:228:CYS:SG	2:B:36:VAL:HG21	2.27	0.75
1:A:79:VAL:O	1:A:83:ILE:HG13	1.86	0.75
1:A:234:PRO:HB2	1:A:357:LYS:CB	2.17	0.75
1:A:75:ILE:HG22	1:A:79:VAL:HG23	1.68	0.75
1:A:103:ASN:HA	1:A:106:LEU:HD12	1.69	0.74
1:A:234:PRO:HB2	1:A:357:LYS:HB2	1.69	0.74
1:A:62:ILE:HD12	1:A:62:ILE:N	1.95	0.74
1:A:33:VAL:HG13	1:A:157:LEU:HD22	1.66	0.74
1:A:63:THR:HG23	1:A:76:GLY:N	2.03	0.74
3:C:36:VAL:O	3:C:39:ALA:HB3	1.88	0.74
1:A:43:ILE:O	1:A:70:LEU:HD13	1.88	0.73
1:A:152:ILE:HD13	1:A:155:ILE:HD12	1.72	0.72
2:B:52:TYR:CE1	2:B:56:VAL:HG21	2.25	0.72
1:A:231:VAL:O	1:A:249:ILE:HG12	1.89	0.71
1:A:102:GLU:O	1:A:106:LEU:HG	1.90	0.71
1:A:15:GLU:OE1	1:A:17:PRO:HG3	1.90	0.71
1:A:195:LYS:HD3	1:A:209:TYR:CE2	2.26	0.70
1:A:377:LEU:HA	2:B:21:VAL:HG11	1.73	0.70
1:A:188:GLY:HA2	2:B:52:TYR:HE1	1.57	0.70
1:A:183:PHE:CE1	2:B:49:ILE:HG13	2.26	0.70
1:A:406:LEU:O	1:A:410:ILE:HG13	1.92	0.69
1:A:274:LEU:O	1:A:277:TYR:HB3	1.91	0.69
1:A:273:GLY:HA2	1:A:284:LEU:HD12	1.74	0.69
1:A:166:ILE:HD13	1:A:418:LEU:CD2	2.23	0.69
1:A:250:LYS:O	1:A:254:VAL:HG12	1.93	0.68
1:A:3:LYS:HA	1:A:3:LYS:HE3	1.74	0.68
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.59	0.68
1:A:16:LEU:HD23	1:A:16:LEU:N	2.05	0.68
1:A:256:ASN:N	1:A:258:PRO:HD2	2.07	0.67
1:A:152:ILE:HA	1:A:155:ILE:HD12	1.76	0.67
1:A:231:VAL:HB	1:A:249:ILE:HG13	1.77	0.67
1:A:257:ILE:HG22	1:A:258:PRO:HD3	1.76	0.67
1:A:80:THR:HA	1:A:83:ILE:HD12	1.76	0.67
1:A:273:GLY:CA	1:A:284:LEU:HD12	2.25	0.67
1:A:408:VAL:HG13	2:B:40:THR:CG2	2.25	0.67
1:A:360:ARG:HB3	1:A:365:ALA:HB1	1.77	0.66
1:A:250:LYS:HD2	1:A:253:TYR:CD2	2.29	0.66
1:A:254:VAL:HG22	1:A:255:SER:N	2.11	0.66
1:A:85:MET:HE2	1:A:111:GLN:HB2	1.76	0.66
1:A:231:VAL:HB	1:A:249:ILE:CG1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ILE:O	1:A:313:PRO:HD3	1.96	0.66
1:A:268:ASN:O	1:A:272:TRP:HB2	1.95	0.66
1:A:151:SER:O	1:A:155:ILE:HG13	1.95	0.66
1:A:29:TRP:NE1	1:A:164:TYR:HD2	1.94	0.65
1:A:257:ILE:HG21	1:A:334:TRP:CH2	2.32	0.65
1:A:84:ILE:O	1:A:87:LEU:HB2	1.96	0.65
1:A:344:SER:O	1:A:346:ALA:N	2.30	0.65
1:A:358:GLY:O	1:A:359:PHE:HB2	1.96	0.65
1:A:270:GLN:NE2	1:A:301:SER:HB3	2.11	0.64
1:A:86:GLN:O	1:A:333:PHE:HD2	1.80	0.64
1:A:391:ILE:O	1:A:395:ILE:HG22	1.98	0.64
1:A:251:PHE:CE1	1:A:381:SER:HA	2.33	0.64
1:A:317:ILE:O	1:A:321:ILE:HG13	1.97	0.64
1:A:320:MET:O	1:A:324:ILE:HG12	1.98	0.63
1:A:13:GLU:HG3	1:A:14:VAL:N	2.10	0.63
1:A:52:ILE:HG23	1:A:132:PHE:HA	1.80	0.63
1:A:166:ILE:HD13	1:A:418:LEU:HD21	1.80	0.63
1:A:65:SER:O	1:A:66:ARG:HB2	1.96	0.63
1:A:149:PHE:HD2	3:C:40:PHE:HZ	1.45	0.62
2:B:29:THR:O	2:B:32:GLU:N	2.31	0.62
1:A:219:VAL:HG12	1:A:220:PHE:N	2.14	0.62
1:A:392:ALA:O	1:A:395:ILE:HG23	2.00	0.62
1:A:35:VAL:HG13	2:B:54:ILE:HD11	1.81	0.62
1:A:88:LEU:C	1:A:90:GLY:H	2.03	0.62
1:A:164:TYR:CE1	3:C:30:PRO:HG2	2.35	0.61
2:B:35:ALA:O	2:B:39:VAL:HG12	2.00	0.61
1:A:23:PHE:HE1	1:A:421:GLU:HB2	1.65	0.61
1:A:244:VAL:HG12	1:A:245:GLY:H	1.64	0.61
1:A:281:ILE:N	1:A:281:ILE:HD12	2.15	0.61
1:A:5:ILE:N	1:A:6:PRO:HD2	2.15	0.61
1:A:345:MET:O	1:A:349:ILE:HG13	2.01	0.61
1:A:388:LEU:O	1:A:391:ILE:HG22	2.01	0.61
2:B:46:LEU:HD11	2:B:50:ILE:HD11	1.81	0.61
1:A:188:GLY:HA2	2:B:52:TYR:CE1	2.36	0.61
2:B:64:ILE:O	2:B:65:LEU:HD23	2.01	0.60
1:A:136:THR:HB	1:A:139:LEU:HB3	1.82	0.60
1:A:75:ILE:HG22	1:A:79:VAL:CG2	2.30	0.60
1:A:157:LEU:HA	1:A:160:ILE:HD12	1.83	0.60
1:A:5:ILE:HG22	1:A:9:GLU:CD	2.22	0.60
1:A:325:ILE:HG13	1:A:326:THR:N	2.17	0.60
1:A:55:ILE:HG22	1:A:67:ILE:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:HB1	1:A:274:LEU:HD12	1.82	0.60
1:A:255:SER:HA	1:A:258:PRO:HG2	1.83	0.59
1:A:344:SER:C	1:A:346:ALA:H	2.06	0.59
1:A:257:ILE:HG22	1:A:258:PRO:CD	2.32	0.59
1:A:83:ILE:HG21	1:A:265:LEU:HD23	1.84	0.59
1:A:100:ILE:HG22	1:A:102:GLU:H	1.67	0.59
1:A:93:ILE:HG22	1:A:94:ILE:HG13	1.84	0.59
1:A:388:LEU:HD23	1:A:405:LEU:CD1	2.32	0.59
1:A:3:LYS:C	1:A:5:ILE:H	2.06	0.59
1:A:393:ASN:HD21	1:A:402:THR:HG22	1.68	0.59
1:A:11:ILE:HD11	1:A:113:LEU:CD2	2.27	0.59
1:A:88:LEU:O	1:A:90:GLY:N	2.36	0.59
1:A:255:SER:OG	1:A:382:SER:HB3	2.03	0.59
1:A:52:ILE:N	1:A:52:ILE:HD12	2.18	0.58
1:A:405:LEU:O	1:A:406:LEU:C	2.41	0.58
1:A:43:ILE:HB	1:A:70:LEU:HD22	1.84	0.58
1:A:251:PHE:CD1	1:A:251:PHE:O	2.56	0.58
3:C:30:PRO:O	3:C:34:ILE:HG12	2.03	0.58
1:A:34:LEU:O	1:A:37:TYR:HB3	2.04	0.58
1:A:152:ILE:HA	1:A:155:ILE:CD1	2.33	0.58
1:A:211:ALA:HB3	1:A:212:PRO:CD	2.33	0.58
1:A:231:VAL:HB	1:A:249:ILE:HD11	1.85	0.58
1:A:355:ALA:HB2	1:A:361:LYS:HA	1.85	0.58
1:A:166:ILE:HG22	1:A:167:GLY:H	1.69	0.58
2:B:4:PHE:O	2:B:8:ILE:HG13	2.03	0.58
1:A:257:ILE:N	1:A:258:PRO:CD	2.66	0.58
1:A:200:LEU:HD23	1:A:205:PRO:HG3	1.85	0.58
1:A:299:TYR:C	1:A:300:LEU:HD23	2.24	0.58
1:A:135:LEU:H	1:A:135:LEU:HD12	1.68	0.57
1:A:23:PHE:CD1	1:A:421:GLU:HB3	2.39	0.57
1:A:135:LEU:O	1:A:137:PRO:HD3	2.04	0.57
1:A:373:TYR:O	1:A:376:PRO:HG2	2.04	0.57
1:A:393:ASN:HD21	1:A:402:THR:N	2.03	0.57
1:A:30:THR:O	1:A:33:VAL:HG23	2.05	0.57
3:C:32:HIS:O	3:C:36:VAL:HG23	2.05	0.57
1:A:85:MET:HE1	1:A:111:GLN:N	2.20	0.57
1:A:344:SER:C	1:A:346:ALA:N	2.55	0.57
1:A:80:THR:O	1:A:83:ILE:HB	2.05	0.57
1:A:12:PRO:HB3	3:C:28:VAL:HG21	1.87	0.57
1:A:374:ILE:CB	1:A:375:PRO:HD3	2.35	0.57
1:A:279:MET:HG2	1:A:279:MET:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLY:HA2	1:A:417:GLN:NE2	2.20	0.56
2:B:16:GLU:O	2:B:20:ARG:HD3	2.04	0.56
1:A:147:ILE:HG22	1:A:148:ALA:N	2.20	0.56
1:A:141:PHE:CZ	1:A:145:ILE:HD11	2.40	0.56
1:A:257:ILE:HG21	1:A:334:TRP:CZ2	2.40	0.56
1:A:189:PRO:C	1:A:191:GLY:H	2.09	0.56
1:A:98:LEU:O	1:A:99:SER:C	2.43	0.56
1:A:156:TYR:O	1:A:160:ILE:HG13	2.06	0.56
1:A:356:ILE:HG22	1:A:357:LYS:N	2.21	0.56
1:A:405:LEU:HD23	1:A:406:LEU:N	2.21	0.56
1:A:116:ILE:H	1:A:116:ILE:HD12	1.71	0.56
1:A:13:GLU:CG	1:A:14:VAL:H	2.15	0.55
1:A:98:LEU:O	1:A:100:ILE:O	2.24	0.55
2:B:18:CYS:O	2:B:21:VAL:N	2.38	0.55
1:A:410:ILE:O	1:A:414:MET:HB2	2.05	0.55
1:A:231:VAL:HB	1:A:249:ILE:CD1	2.35	0.55
1:A:146:GLN:HE21	3:C:44:GLU:HG2	1.72	0.55
1:A:206:ASN:OD1	1:A:208:GLU:HB2	2.07	0.54
1:A:273:GLY:HA3	1:A:287:TYR:OH	2.07	0.54
1:A:374:ILE:HB	1:A:375:PRO:CD	2.36	0.54
1:A:254:VAL:CG2	1:A:255:SER:N	2.70	0.54
1:A:112:LYS:O	1:A:116:ILE:HD12	2.07	0.54
1:A:23:PHE:HD1	1:A:421:GLU:HB3	1.72	0.54
1:A:308:SER:HB3	1:A:394:PHE:O	2.07	0.54
2:B:56:VAL:HG12	2:B:57:PRO:N	2.23	0.54
1:A:293:VAL:HG12	1:A:293:VAL:O	2.07	0.54
1:A:142:LEU:O	1:A:145:ILE:HB	2.08	0.54
1:A:368:HIS:O	1:A:370:LEU:N	2.41	0.54
1:A:384:PHE:O	1:A:387:PHE:HB3	2.08	0.54
1:A:189:PRO:HD3	2:B:56:VAL:CG2	2.28	0.54
1:A:18:VAL:HG12	1:A:18:VAL:O	2.08	0.54
1:A:304:TYR:HD1	1:A:305:GLY:N	2.06	0.54
1:A:149:PHE:HB3	3:C:40:PHE:CE2	2.43	0.54
1:A:4:LEU:C	1:A:6:PRO:HD2	2.28	0.54
1:A:63:THR:HG23	1:A:76:GLY:CA	2.38	0.53
1:A:75:ILE:HD11	1:A:173:PHE:CD1	2.43	0.53
1:A:149:PHE:HB3	3:C:40:PHE:CZ	2.43	0.53
1:A:405:LEU:C	1:A:405:LEU:HD23	2.29	0.53
1:A:155:ILE:O	1:A:159:GLU:HG2	2.09	0.53
1:A:374:ILE:O	1:A:377:LEU:N	2.41	0.53
1:A:152:ILE:HD13	1:A:155:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ILE:O	1:A:335:VAL:HB	2.08	0.53
1:A:224:VAL:HG12	2:B:33:TYR:HE1	1.74	0.53
2:B:49:ILE:HG22	2:B:50:ILE:N	2.24	0.53
1:A:287:TYR:CE2	1:A:292:ALA:HB2	2.44	0.52
1:A:234:PRO:CB	1:A:357:LYS:HB2	2.36	0.52
1:A:83:ILE:HG23	1:A:330:PHE:CZ	2.44	0.52
1:A:206:ASN:HB3	1:A:209:TYR:HD1	1.74	0.52
1:A:92:GLY:O	1:A:94:ILE:N	2.42	0.52
1:A:333:PHE:CD1	1:A:333:PHE:N	2.77	0.52
1:A:172:LEU:C	1:A:172:LEU:HD23	2.30	0.52
1:A:256:ASN:C	1:A:258:PRO:HD2	2.30	0.52
1:A:333:PHE:HD1	1:A:333:PHE:N	2.07	0.52
1:A:5:ILE:HG22	1:A:9:GLU:OE1	2.10	0.52
1:A:384:PHE:O	1:A:385:VAL:C	2.47	0.52
1:A:389:ALA:O	1:A:392:ALA:HB3	2.09	0.52
1:A:88:LEU:C	1:A:90:GLY:N	2.63	0.52
1:A:244:VAL:CG1	1:A:245:GLY:N	2.67	0.52
1:A:166:ILE:HG22	1:A:167:GLY:N	2.25	0.52
1:A:287:TYR:HB3	1:A:291:ARG:O	2.09	0.52
1:A:108:GLN:O	1:A:109:GLY:C	2.47	0.52
2:B:52:TYR:CE1	2:B:56:VAL:CG2	2.93	0.51
1:A:72:THR:HB	1:A:147:ILE:HD12	1.92	0.51
2:B:21:VAL:C	2:B:23:LEU:H	2.13	0.51
1:A:417:GLN:O	1:A:421:GLU:HG2	2.11	0.51
1:A:388:LEU:HD23	1:A:405:LEU:HD12	1.91	0.51
1:A:402:THR:O	1:A:405:LEU:HB3	2.11	0.51
1:A:252:VAL:HG23	1:A:253:TYR:H	1.75	0.51
1:A:113:LEU:O	1:A:116:ILE:N	2.43	0.51
1:A:98:LEU:O	1:A:100:ILE:N	2.43	0.51
1:A:164:TYR:CZ	3:C:30:PRO:HG2	2.46	0.51
1:A:347:LYS:O	1:A:351:SER:N	2.39	0.51
1:A:136:THR:HG22	1:A:139:LEU:H	1.76	0.51
1:A:314:ILE:O	1:A:318:VAL:HG23	2.11	0.51
1:A:425:GLU:O	1:A:425:GLU:HG3	2.11	0.51
1:A:21:ILE:H	1:A:21:ILE:HD12	1.76	0.51
3:C:22:THR:HG22	3:C:24:SER:H	1.76	0.51
1:A:172:LEU:C	1:A:172:LEU:CD2	2.80	0.50
1:A:232:GLU:O	1:A:233:ILE:HD13	2.11	0.50
1:A:24:LYS:O	1:A:28:LYS:HG3	2.11	0.50
1:A:250:LYS:NZ	1:A:416:GLU:OE1	2.34	0.50
2:B:14:PHE:O	2:B:17:GLU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:PHE:HE1	2:B:49:ILE:HG13	1.76	0.50
1:A:102:GLU:C	1:A:106:LEU:HG	2.32	0.50
1:A:43:ILE:HG22	1:A:70:LEU:HD11	1.93	0.50
1:A:293:VAL:O	1:A:294:ASP:HB2	2.11	0.50
3:C:30:PRO:HA	3:C:33:VAL:CG2	2.42	0.50
1:A:82:GLY:O	1:A:86:GLN:HG2	2.11	0.50
1:A:274:LEU:C	1:A:274:LEU:HD13	2.32	0.50
1:A:253:TYR:HE1	1:A:413:ARG:HH11	1.60	0.50
1:A:370:LEU:O	1:A:371:LYS:C	2.50	0.50
1:A:361:LYS:HB3	1:A:361:LYS:NZ	2.27	0.49
1:A:75:ILE:HG21	1:A:170:ILE:HG23	1.93	0.49
1:A:15:GLU:O	1:A:17:PRO:HD3	2.12	0.49
1:A:299:TYR:O	1:A:300:LEU:HD23	2.12	0.49
1:A:382:SER:O	1:A:383:ALA:C	2.50	0.49
2:B:49:ILE:O	2:B:52:TYR:HB3	2.13	0.49
1:A:67:ILE:HG23	1:A:72:THR:HG23	1.94	0.49
1:A:310:ILE:O	1:A:312:ASP:N	2.38	0.49
2:B:29:THR:O	2:B:30:LYS:C	2.50	0.49
1:A:35:VAL:HG13	2:B:54:ILE:CD1	2.42	0.49
1:A:75:ILE:O	1:A:79:VAL:HG23	2.13	0.49
1:A:116:ILE:HD12	1:A:116:ILE:N	2.26	0.49
1:A:46:TYR:CB	1:A:146:GLN:HE22	2.19	0.49
1:A:160:ILE:HD11	3:C:33:VAL:CG2	2.43	0.49
1:A:340:LEU:H	1:A:340:LEU:CD1	2.19	0.49
1:A:89:VAL:HG12	1:A:89:VAL:O	2.12	0.49
1:A:255:SER:C	1:A:258:PRO:HD2	2.32	0.49
1:A:29:TRP:CE2	1:A:164:TYR:HD2	2.30	0.49
1:A:14:VAL:HG21	1:A:159:GLU:HB3	1.95	0.48
1:A:314:ILE:HD12	1:A:315:HIS:N	2.19	0.48
1:A:219:VAL:HG13	1:A:223:VAL:CG2	2.42	0.48
1:A:356:ILE:HG22	1:A:357:LYS:H	1.78	0.48
1:A:75:ILE:HD11	1:A:173:PHE:HD1	1.78	0.48
2:B:55:HIS:O	2:B:56:VAL:C	2.51	0.48
1:A:153:ILE:HG21	3:C:37:THR:HG23	1.96	0.48
1:A:374:ILE:O	1:A:377:LEU:HB3	2.13	0.48
2:B:32:GLU:O	2:B:35:ALA:HB3	2.14	0.48
1:A:359:PHE:N	1:A:369:ARG:NH2	2.62	0.48
1:A:92:GLY:O	1:A:95:GLN:HG3	2.14	0.48
1:A:123:ALA:HB2	1:A:148:ALA:HB2	1.96	0.48
1:A:118:MET:O	1:A:122:GLU:HG2	2.13	0.48
3:C:34:ILE:O	3:C:38:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:HG21	1:A:107:PHE:CD1	2.47	0.48
1:A:306:LEU:HD12	1:A:306:LEU:N	2.29	0.48
3:C:35:GLY:HA2	3:C:38:VAL:HG23	1.95	0.48
1:A:167:GLY:HA2	1:A:417:GLN:CD	2.34	0.48
1:A:384:PHE:O	1:A:387:PHE:N	2.47	0.48
1:A:214:ILE:O	1:A:215:GLY:C	2.52	0.48
1:A:302:THR:HG21	1:A:393:ASN:OD1	2.14	0.48
1:A:388:LEU:HD23	1:A:405:LEU:HD11	1.96	0.48
1:A:34:LEU:HD13	1:A:172:LEU:HD21	1.96	0.48
1:A:23:PHE:CE1	1:A:421:GLU:HB2	2.48	0.48
1:A:124:VAL:HA	1:A:144:ILE:CD1	2.44	0.47
1:A:419:LEU:C	1:A:421:GLU:N	2.65	0.47
1:A:136:THR:O	1:A:138:LEU:N	2.47	0.47
1:A:294:ASP:N	1:A:298:TYR:HB2	2.29	0.47
1:A:266:PHE:HD1	1:A:266:PHE:H	1.62	0.47
1:A:94:ILE:O	1:A:94:ILE:HG22	2.14	0.47
1:A:84:ILE:O	1:A:87:LEU:N	2.47	0.47
1:A:400:GLY:O	1:A:401:GLY:C	2.53	0.47
1:A:240:ILE:CG2	1:A:241:LYS:H	2.02	0.47
2:B:18:CYS:O	2:B:19:ARG:C	2.53	0.47
1:A:252:VAL:HG23	1:A:253:TYR:N	2.29	0.47
2:B:19:ARG:O	2:B:23:LEU:HD12	2.15	0.47
1:A:311:SER:O	1:A:312:ASP:CG	2.53	0.47
1:A:172:LEU:CD2	1:A:176:ALA:HB2	2.45	0.47
1:A:240:ILE:O	1:A:241:LYS:HG3	2.14	0.47
1:A:118:MET:O	1:A:122:GLU:CG	2.63	0.47
1:A:323:MET:O	1:A:324:ILE:C	2.52	0.47
1:A:429:ALA:O	1:A:431:ALA:N	2.39	0.47
1:A:38:PHE:CD1	2:B:51:GLY:HA2	2.49	0.47
1:A:171:GLY:HA3	1:A:413:ARG:HH21	1.80	0.47
1:A:120:PHE:O	1:A:123:ALA:HB3	2.15	0.47
1:A:98:LEU:HD23	1:A:103:ASN:HB3	1.96	0.47
1:A:86:GLN:O	1:A:90:GLY:HA3	2.13	0.47
1:A:194:TRP:O	1:A:195:LYS:C	2.52	0.47
1:A:314:ILE:CD1	1:A:315:HIS:H	2.21	0.47
2:B:23:LEU:C	2:B:25:LEU:H	2.18	0.47
2:B:36:VAL:O	2:B:37:ALA:C	2.53	0.46
1:A:136:THR:O	1:A:137:PRO:C	2.54	0.46
1:A:16:LEU:CD2	1:A:16:LEU:H	2.06	0.46
1:A:287:TYR:CD2	1:A:292:ALA:HB2	2.50	0.46
1:A:67:ILE:CA	1:A:72:THR:HG23	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:O	1:A:278:ARG:HD3	2.15	0.46
1:A:224:VAL:HG12	2:B:33:TYR:CE1	2.51	0.46
1:A:74:GLY:O	1:A:77:PRO:HD2	2.14	0.46
1:A:87:LEU:HD21	1:A:329:MET:HE1	1.96	0.46
1:A:98:LEU:CA	1:A:103:ASN:HB2	2.34	0.46
1:A:304:TYR:CD1	1:A:305:GLY:N	2.84	0.46
1:A:338:THR:HG22	1:A:339:GLY:N	2.31	0.46
1:A:8:LEU:HD23	1:A:8:LEU:C	2.36	0.46
1:A:12:PRO:HB3	3:C:28:VAL:CG2	2.45	0.46
1:A:181:THR:HG21	1:A:399:GLY:HA2	1.96	0.46
1:A:153:ILE:HD11	3:C:40:PHE:CD1	2.50	0.46
2:B:61:ILE:O	2:B:62:LYS:C	2.52	0.46
2:B:6:GLN:NE2	2:B:9:GLU:OE1	2.49	0.46
1:A:366:ILE:O	1:A:367:GLU:C	2.53	0.46
1:A:374:ILE:CB	1:A:375:PRO:CD	2.93	0.46
1:A:135:LEU:N	1:A:135:LEU:HD12	2.30	0.46
1:A:79:VAL:HG11	1:A:264:ALA:CB	2.45	0.45
1:A:195:LYS:HB3	1:A:209:TYR:CE2	2.50	0.45
1:A:14:VAL:HG13	3:C:30:PRO:HG3	1.98	0.45
1:A:166:ILE:CD1	1:A:418:LEU:HD21	2.45	0.45
1:A:359:PHE:O	1:A:360:ARG:HB2	2.16	0.45
1:A:242:GLY:O	1:A:244:VAL:HG23	2.16	0.45
1:A:91:SER:C	1:A:93:ILE:H	2.20	0.45
1:A:189:PRO:CD	2:B:56:VAL:HG22	2.31	0.45
1:A:112:LYS:HD3	1:A:116:ILE:HD11	1.98	0.45
1:A:11:ILE:CD1	1:A:113:LEU:HD23	2.32	0.45
1:A:63:THR:HG22	1:A:63:THR:O	2.16	0.45
3:C:49:TYR:CD1	3:C:49:TYR:N	2.83	0.45
1:A:244:VAL:O	1:A:245:GLY:O	2.35	0.45
1:A:129:ALA:C	1:A:278:ARG:HD3	2.37	0.45
1:A:45:VAL:HG11	1:A:147:ILE:HD11	1.98	0.45
1:A:312:ASP:N	1:A:313:PRO:HD3	2.32	0.45
1:A:265:LEU:HD22	1:A:265:LEU:HA	1.84	0.45
2:B:10:GLN:O	2:B:13:GLU:N	2.49	0.45
1:A:83:ILE:HG23	1:A:330:PHE:CE2	2.51	0.45
1:A:77:PRO:O	1:A:80:THR:N	2.50	0.45
1:A:3:LYS:O	1:A:5:ILE:N	2.48	0.45
1:A:170:ILE:O	1:A:171:GLY:C	2.56	0.44
1:A:172:LEU:O	1:A:175:ALA:N	2.50	0.44
1:A:153:ILE:CD1	3:C:37:THR:HG23	2.40	0.44
1:A:359:PHE:H	1:A:369:ARG:NH2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HD13	1:A:418:LEU:HD23	1.97	0.44
3:C:30:PRO:O	3:C:33:VAL:HG23	2.17	0.44
1:A:337:THR:OG1	1:A:338:THR:N	2.51	0.44
1:A:342:PRO:HG2	1:A:371:LYS:HA	2.00	0.44
1:A:247:TYR:C	1:A:247:TYR:CD1	2.91	0.44
1:A:143:VAL:O	1:A:144:ILE:C	2.56	0.44
1:A:194:TRP:O	1:A:196:PHE:N	2.51	0.44
1:A:404:VAL:O	1:A:408:VAL:HG23	2.17	0.44
1:A:405:LEU:CD2	1:A:406:LEU:N	2.81	0.44
1:A:194:TRP:O	1:A:197:LEU:N	2.50	0.44
1:A:130:GLY:HA3	1:A:278:ARG:NH1	2.33	0.44
2:B:4:PHE:CD2	2:B:8:ILE:HD11	2.53	0.44
1:A:117:ILE:O	1:A:121:VAL:HG23	2.17	0.44
1:A:216:THR:OG1	1:A:398:LEU:HB3	2.18	0.44
1:A:259:VAL:CG1	1:A:406:LEU:HD21	2.48	0.43
1:A:349:ILE:HG22	1:A:354:MET:O	2.18	0.43
1:A:171:GLY:HA2	1:A:410:ILE:HD13	2.00	0.43
1:A:312:ASP:O	1:A:313:PRO:C	2.56	0.43
1:A:393:ASN:ND2	1:A:402:THR:H	2.10	0.43
1:A:14:VAL:CG1	3:C:30:PRO:HG3	2.48	0.43
1:A:340:LEU:HD12	1:A:340:LEU:N	2.23	0.43
1:A:69:THR:C	1:A:71:ILE:H	2.22	0.43
1:A:230:ARG:NH1	1:A:230:ARG:HG3	2.28	0.43
1:A:304:TYR:C	1:A:304:TYR:CD1	2.91	0.43
1:A:225:TYR:C	1:A:225:TYR:CD2	2.92	0.43
3:C:30:PRO:HA	3:C:33:VAL:HG22	2.00	0.43
1:A:256:ASN:C	1:A:258:PRO:CD	2.87	0.43
1:A:362:SER:HB2	1:A:365:ALA:HB2	2.01	0.43
1:A:49:GLY:C	1:A:51:GLN:H	2.22	0.43
1:A:169:GLY:O	1:A:170:ILE:C	2.56	0.43
1:A:80:THR:HG23	1:A:268:ASN:HD21	1.76	0.43
1:A:149:PHE:CD2	3:C:40:PHE:HZ	2.31	0.43
3:C:31:GLU:OE2	3:C:31:GLU:N	2.37	0.43
1:A:392:ALA:O	1:A:395:ILE:CG2	2.65	0.43
1:A:23:PHE:CE1	1:A:421:GLU:CB	3.02	0.43
1:A:361:LYS:HB3	1:A:361:LYS:HZ2	1.83	0.43
1:A:29:TRP:O	1:A:30:THR:C	2.57	0.43
1:A:13:GLU:O	3:C:28:VAL:HB	2.18	0.43
1:A:302:THR:HA	1:A:303:PRO:HD3	1.73	0.42
1:A:163:LYS:O	1:A:164:TYR:CD1	2.72	0.42
1:A:224:VAL:O	1:A:225:TYR:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:O	1:A:334:TRP:HB3	2.19	0.42
1:A:171:GLY:O	1:A:410:ILE:HG21	2.19	0.42
1:A:46:TYR:HB3	1:A:146:GLN:NE2	2.20	0.42
1:A:277:TYR:C	1:A:279:MET:H	2.22	0.42
1:A:418:LEU:HA	1:A:418:LEU:HD23	1.88	0.42
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.94	0.42
2:B:14:PHE:C	2:B:14:PHE:CD1	2.91	0.42
2:B:66:LYS:HB2	2:B:66:LYS:NZ	2.34	0.42
2:B:64:ILE:O	2:B:64:ILE:HG23	2.19	0.42
1:A:257:ILE:HG22	1:A:258:PRO:N	2.35	0.42
3:C:43:ILE:O	3:C:47:LEU:N	2.44	0.42
1:A:79:VAL:HG11	1:A:264:ALA:HB2	2.01	0.42
1:A:85:MET:HG3	1:A:111:GLN:HG3	2.02	0.42
1:A:38:PHE:CE1	2:B:51:GLY:N	2.87	0.42
1:A:244:VAL:CG1	1:A:245:GLY:H	2.24	0.42
1:A:92:GLY:O	1:A:93:ILE:C	2.58	0.42
1:A:385:VAL:HG12	1:A:386:GLY:N	2.35	0.42
1:A:193:LEU:HG	1:A:197:LEU:HD22	2.02	0.42
1:A:281:ILE:HA	1:A:282:PRO:HD3	1.90	0.42
1:A:337:THR:O	1:A:338:THR:C	2.58	0.42
1:A:116:ILE:HA	1:A:119:CYS:HB2	2.02	0.42
1:A:100:ILE:C	1:A:102:GLU:N	2.73	0.42
2:B:14:PHE:HE1	2:B:18:CYS:SG	2.43	0.42
1:A:166:ILE:CG2	1:A:417:GLN:HG2	2.50	0.42
1:A:247:TYR:C	1:A:247:TYR:HD1	2.24	0.42
1:A:179:SER:OG	2:B:44:ILE:CG2	2.68	0.41
2:B:14:PHE:CE1	2:B:18:CYS:SG	3.13	0.41
2:B:15:ILE:O	2:B:18:CYS:HB2	2.20	0.41
1:A:166:ILE:HG22	1:A:417:GLN:HG2	2.02	0.41
2:B:16:GLU:OE2	2:B:16:GLU:HA	2.20	0.41
1:A:329:MET:O	1:A:331:GLY:N	2.53	0.41
1:A:156:TYR:HB3	3:C:33:VAL:HG11	2.02	0.41
1:A:194:TRP:C	1:A:196:PHE:N	2.71	0.41
2:B:40:THR:O	2:B:44:ILE:HG13	2.20	0.41
2:B:3:ASP:O	2:B:6:GLN:HB2	2.20	0.41
1:A:33:VAL:HG11	1:A:161:VAL:CG2	2.50	0.41
1:A:98:LEU:HD22	1:A:104:ARG:HA	2.02	0.41
1:A:149:PHE:O	1:A:152:ILE:HB	2.20	0.41
1:A:415:TYR:CD2	2:B:39:VAL:HG21	2.55	0.41
1:A:31:GLY:O	1:A:35:VAL:HG23	2.20	0.41
1:A:216:THR:HA	1:A:397:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:HG23	1:A:321:ILE:HD11	2.03	0.41
1:A:67:ILE:HG23	1:A:72:THR:CG2	2.50	0.41
2:B:62:LYS:O	2:B:66:LYS:HB2	2.21	0.41
2:B:35:ALA:O	2:B:38:LYS:HB2	2.21	0.41
2:B:4:PHE:CE2	2:B:8:ILE:HD11	2.56	0.41
1:A:256:ASN:O	1:A:257:ILE:C	2.59	0.41
2:B:57:PRO:O	2:B:60:TYR:N	2.54	0.41
1:A:379:VAL:O	1:A:380:MET:C	2.58	0.41
1:A:135:LEU:O	1:A:137:PRO:CD	2.69	0.41
1:A:368:HIS:C	1:A:370:LEU:N	2.74	0.41
1:A:173:PHE:O	1:A:176:ALA:HB3	2.20	0.41
1:A:219:VAL:O	1:A:220:PHE:C	2.59	0.41
1:A:79:VAL:O	1:A:80:THR:C	2.58	0.41
2:B:61:ILE:O	2:B:63:GLY:N	2.54	0.41
1:A:5:ILE:N	1:A:6:PRO:CD	2.83	0.41
2:B:30:LYS:HA	2:B:30:LYS:HD3	1.95	0.41
1:A:238:GLY:O	1:A:239:ARG:HB2	2.21	0.41
1:A:26:LYS:HA	1:A:165:GLY:HA2	2.03	0.41
1:A:124:VAL:HA	1:A:144:ILE:HD11	2.02	0.40
1:A:322:ALA:O	1:A:325:ILE:HG12	2.20	0.40
1:A:393:ASN:O	1:A:394:PHE:C	2.60	0.40
1:A:87:LEU:HD21	1:A:329:MET:CE	2.51	0.40
1:A:89:VAL:HG21	1:A:107:PHE:HD1	1.86	0.40
2:B:10:GLN:O	2:B:13:GLU:HB2	2.22	0.40
1:A:253:TYR:O	1:A:253:TYR:CG	2.75	0.40
1:A:75:ILE:O	1:A:75:ILE:HG22	2.21	0.40
1:A:240:ILE:C	1:A:241:LYS:HG3	2.42	0.40
1:A:417:GLN:HB2	1:A:417:GLN:HE21	1.53	0.40
1:A:189:PRO:C	1:A:191:GLY:N	2.75	0.40
1:A:155:ILE:H	1:A:155:ILE:HG13	1.61	0.40
1:A:43:ILE:C	1:A:70:LEU:HD13	2.41	0.40
1:A:345:MET:O	1:A:349:ILE:CG1	2.69	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	430/436 (99%)	256 (60%)	124 (29%)	50 (12%)	0	7
2	B	63/74 (85%)	38 (60%)	19 (30%)	6 (10%)	1	10
3	C	30/53 (57%)	19 (63%)	11 (37%)	0	100	100
All	All	523/563 (93%)	313 (60%)	154 (29%)	56 (11%)	0	8

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	99	SER
1	A	240	ILE
1	A	311	SER
1	A	329	MET
1	A	338	THR
1	A	346	ALA
1	A	374	ILE
2	B	30	LYS
2	B	55	HIS
1	A	58	PHE
1	A	89	VAL
1	A	93	ILE
1	A	147	ILE
1	A	170	ILE
1	A	172	LEU
1	A	188	GLY
1	A	189	PRO
1	A	244	VAL
1	A	245	GLY
1	A	304	TYR
1	A	345	MET
1	A	360	ARG
1	A	369	ARG
1	A	385	VAL
1	A	405	LEU
1	A	430	ILE
2	B	38	LYS
1	A	4	LEU
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	145	ILE
1	A	205	PRO
1	A	246	LYS
1	A	250	LYS
1	A	288	GLU
1	A	324	ILE
1	A	339	GLY
1	A	429	ALA
2	B	22	TRP
2	B	24	VAL
1	A	173	PHE
1	A	287	TYR
1	A	312	ASP
1	A	359	PHE
2	B	56	VAL
1	A	102	GLU
1	A	109	GLY
1	A	313	PRO
1	A	6	PRO
1	A	136	THR
1	A	137	PRO
1	A	211	ALA
1	A	77	PRO
1	A	375	PRO
1	A	396	GLY
1	A	12	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	351/355 (99%)	315 (90%)	36 (10%)	9	40
2	B	57/66 (86%)	53 (93%)	4 (7%)	19	59
3	C	28/45 (62%)	26 (93%)	2 (7%)	18	58
All	All	436/466 (94%)	394 (90%)	42 (10%)	10	43

All (42) 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	29	TRP
1	A	33	VAL
1	A	62	ILE
1	A	80	THR
1	A	112	LYS
1	A	126	PHE
1	A	135	LEU
1	A	172	LEU
1	A	197	LEU
1	A	202	GLN
1	A	210	ILE
1	A	225	TYR
1	A	247	TYR
1	A	248	PRO
1	A	257	ILE
1	A	259	VAL
1	A	265	LEU
1	A	304	TYR
1	A	306	LEU
1	A	314	ILE
1	A	333	PHE
1	A	336	GLU
1	A	340	LEU
1	A	349	ILE
1	A	359	PHE
1	A	363	GLU
1	A	369	ARG
1	A	375	PRO
1	A	380	MET
1	A	381	SER
1	A	402	THR
1	A	417	GLN
2	B	17	GLU
2	B	19	ARG
2	B	30	LYS
2	B	42	LEU
3	C	33	VAL
3	C	51	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	146	GLN
1	A	180	GLN
1	A	268	ASN
1	A	393	ASN
1	A	417	GLN
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 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, 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	432/436 (99%)	0.02	17 (3%) 43 35	37, 115, 194, 198	0
2	B	65/74 (87%)	-0.53	0 100 100	54, 95, 183, 197	0
3	C	32/53 (60%)	-0.15	1 (3%) 52 43	95, 172, 198, 198	0
All	All	529/563 (93%)	-0.06	18 (3%) 49 40	37, 116, 195, 198	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	ALA	4.7
1	A	96	MET	4.6
1	A	284	LEU	4.4
1	A	306	LEU	4.2
1	A	305	GLY	3.9
1	A	132	PHE	3.6
1	A	302	THR	3.6
1	A	304	TYR	3.4
1	A	283	ILE	3.3
1	A	70	LEU	3.1
1	A	427	HIS	2.6
1	A	251	PHE	2.5
1	A	43	ILE	2.4
3	C	23	PHE	2.3
1	A	301	SER	2.3
1	A	276	LEU	2.3
1	A	68	GLY	2.2
1	A	48	ALA	2.1

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 [i](#)

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.