



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:15 pm GMT

PDB ID : 4KJR
Title : Crystal structure of selenium substituted Ca²⁺/H⁺ antiporter protein YfkE
Authors : Wu, M.; Tong, S.; Zheng, L.
Deposited on : 2013-05-03
Resolution : 3.00 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

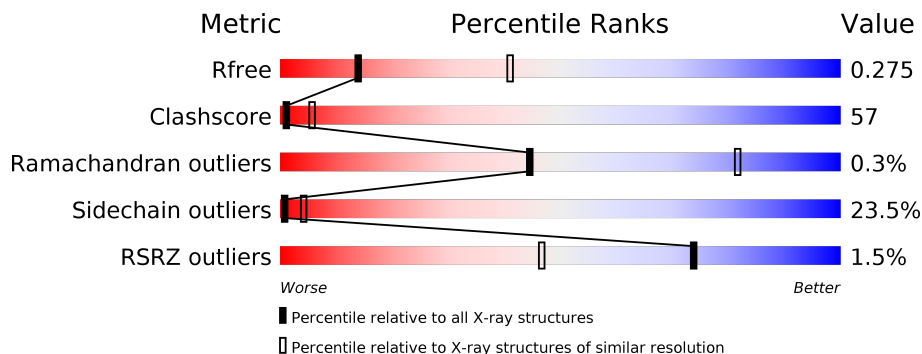
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	351	<div> <div></div> <div> <div></div> <div>39%</div> <div>39%</div> <div>14%</div> <div>7%</div> </div> </div>
1	B	351	<div> <div></div> <div> <div></div> <div>37%</div> <div>39%</div> <div>12%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4785 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 cation exchanger YfkE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	Se	0	0	0
			2441	1628	379	420	2	12			
1	B	311	Total	C	N	O	S	Se	0	0	0
			2332	1560	360	398	2	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MSE	LEU	ENGINEERED MUTATION	UNP O34840
A	116	ALA	LYS	ENGINEERED MUTATION	UNP O34840
B	77	MSE	LEU	ENGINEERED MUTATION	UNP O34840
B	116	ALA	LYS	ENGINEERED MUTATION	UNP O34840

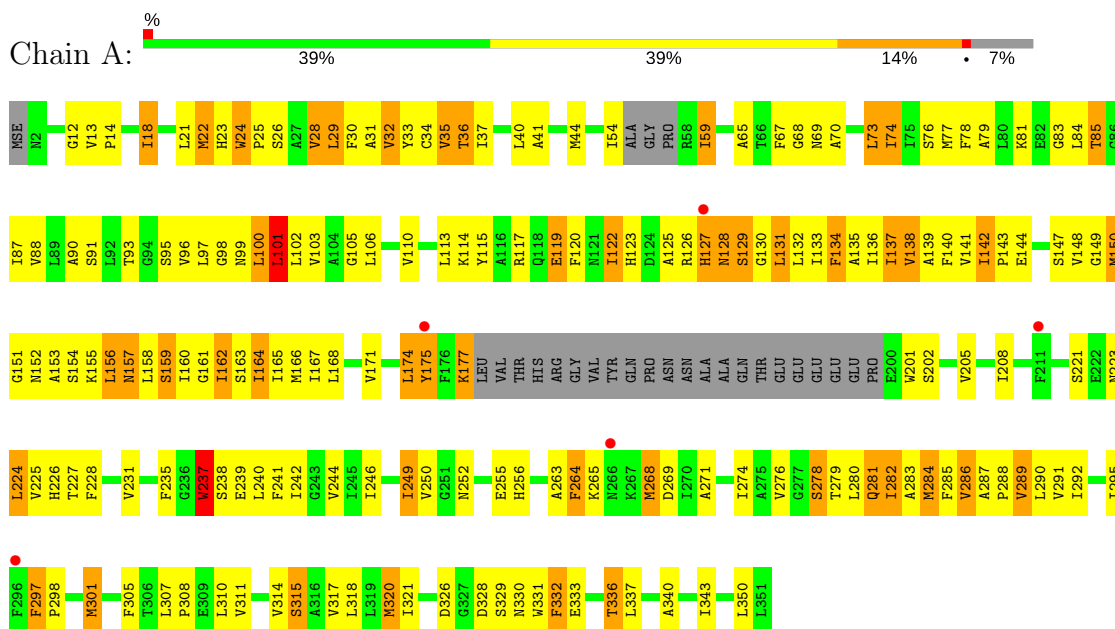
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	4	Total	O	0	0
			4	4		

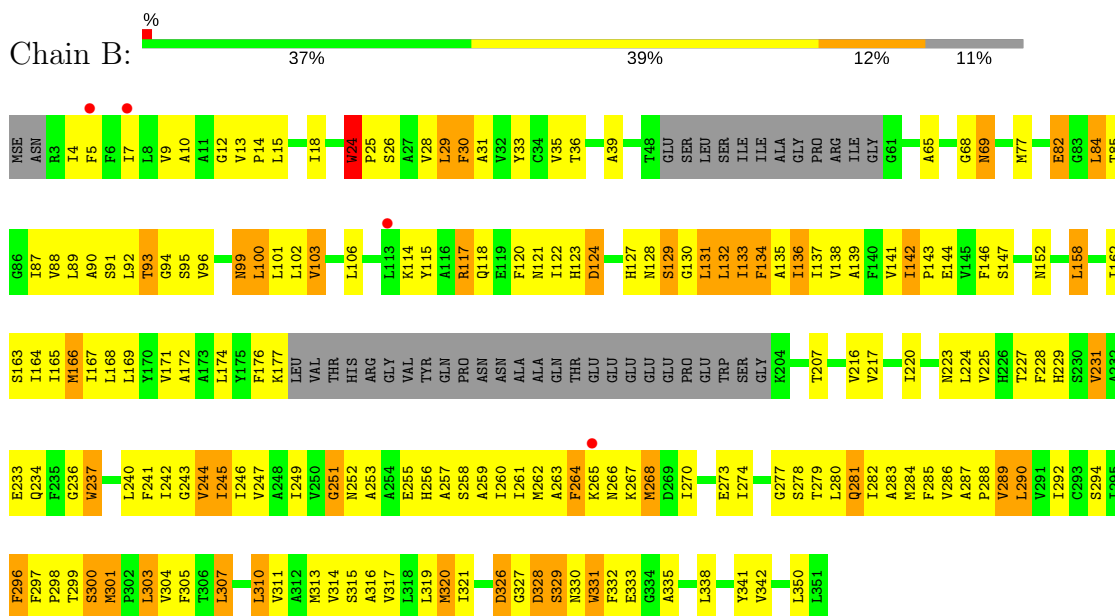
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: cation exchanger YfkE



• Molecule 1: cation exchanger YfkE



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	170.30Å 170.30Å 95.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.16 – 3.00 48.11 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (85.16-3.00) 98.9 (48.11-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.239 , 0.268 0.250 , 0.275	Depositor DCC
R_{free} test set	1058 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	89.6	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 11.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.531 for H, K, L 0.469 for K, H, -L	Depositor
Outliers	0 of 20634 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4785	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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	0.46	4/2478 (0.2%)	0.58	1/3352 (0.0%)
1	B	0.45	1/2367 (0.0%)	0.59	0/3202
All	All	0.46	5/4845 (0.1%)	0.58	1/6554 (0.0%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	TRP	CD2-CE2	5.23	1.47	1.41
1	A	201	TRP	CD2-CE2	5.15	1.47	1.41
1	A	331	TRP	CD2-CE2	5.13	1.47	1.41
1	A	24	TRP	CD2-CE2	5.08	1.47	1.41
1	B	331	TRP	CD2-CE2	5.02	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	LEU	N-CA-C	-5.37	96.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2441	0	2554	304	0
1	B	2332	0	2449	256	0
2	A	8	0	0	0	0
2	B	4	0	0	0	0
All	All	4785	0	5003	559	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 (559) 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:78:PHE:CE2	1:A:225:VAL:HG13	1.20	1.63
1:A:30:PHE:HE1	1:A:228:PHE:CE2	1.25	1.53
1:A:30:PHE:CE1	1:A:228:PHE:CE2	1.95	1.52
1:A:30:PHE:CE1	1:A:228:PHE:HE2	1.24	1.51
1:A:78:PHE:CE2	1:A:225:VAL:CG1	1.95	1.49
1:A:282:ILE:HA	1:A:286:VAL:CG2	1.46	1.43
1:A:164:ILE:CD1	1:A:168:LEU:HD11	1.51	1.38
1:A:78:PHE:CZ	1:A:225:VAL:HG13	1.63	1.32
1:A:127:HIS:O	1:A:131:LEU:CD1	1.78	1.32
1:A:69:ASN:ND2	1:A:281:GLN:OE1	1.64	1.26
1:A:164:ILE:HD13	1:A:168:LEU:CD1	1.69	1.23
1:A:164:ILE:CD1	1:A:168:LEU:CD1	2.17	1.21
1:A:224:LEU:HD13	1:A:228:PHE:HZ	1.05	1.18
1:A:29:LEU:HA	1:A:32:VAL:CG1	1.77	1.14
1:A:156:LEU:HD23	1:A:157:ASN:N	1.62	1.14
1:B:12:GLY:HA3	1:B:36:THR:HG21	1.20	1.14
1:A:282:ILE:CA	1:A:286:VAL:HG23	1.76	1.14
1:B:134:PHE:CE1	1:B:284:MSE:HE3	1.84	1.13
1:A:81:LYS:HE2	1:A:297:PHE:CE1	1.84	1.13
1:A:12:GLY:HA3	1:A:36:THR:HG23	1.20	1.12
1:B:134:PHE:HE1	1:B:284:MSE:CE	1.60	1.12
1:A:33:TYR:OH	1:A:223:ASN:ND2	1.83	1.12
1:B:133:ILE:HD11	1:B:137:ILE:HD12	1.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ASN:HB2	1:B:252:ASN:ND2	1.65	1.12
1:A:127:HIS:O	1:A:131:LEU:HD11	0.95	1.11
1:B:296:PHE:CD2	1:B:297:PHE:CD1	2.39	1.11
1:A:237:TRP:HB2	1:A:238:SER:OG	1.49	1.10
1:B:296:PHE:CE2	1:B:297:PHE:CE1	2.40	1.10
1:B:96:VAL:HG21	1:B:313:MSE:HE3	1.15	1.09
1:A:224:LEU:HD22	1:A:228:PHE:CE2	1.88	1.08
1:B:134:PHE:HE1	1:B:284:MSE:HE3	0.91	1.07
1:A:156:LEU:O	1:A:160:ILE:HG12	1.56	1.06
1:B:24:TRP:H	1:B:25:PRO:CD	1.68	1.06
1:A:30:PHE:HB2	1:A:227:THR:HG21	1.34	1.05
1:B:133:ILE:CD1	1:B:137:ILE:HD12	1.86	1.05
1:B:65:ALA:O	1:B:281:GLN:OE1	1.75	1.04
1:A:224:LEU:HD13	1:A:228:PHE:CZ	1.93	1.04
1:A:26:SER:O	1:A:29:LEU:CD1	2.05	1.04
1:A:131:LEU:H	1:A:131:LEU:HD12	1.20	1.04
1:B:94:GLY:CA	1:B:244:VAL:HG22	1.87	1.03
1:A:26:SER:O	1:A:29:LEU:HD12	1.58	1.02
1:A:164:ILE:HD11	1:A:168:LEU:HD11	1.34	1.02
1:B:96:VAL:HG12	1:B:282:ILE:HG21	1.36	1.02
1:A:30:PHE:CD1	1:A:228:PHE:HE2	1.78	1.01
1:B:134:PHE:CE1	1:B:284:MSE:CE	2.41	1.01
1:B:24:TRP:H	1:B:25:PRO:HD3	1.26	0.99
1:A:282:ILE:HA	1:A:286:VAL:HG21	1.44	0.98
1:A:153:ALA:O	1:A:156:LEU:CD2	2.12	0.98
1:A:282:ILE:HA	1:A:286:VAL:HG23	1.00	0.97
1:A:285:PHE:O	1:A:289:VAL:HG13	1.64	0.97
1:A:101:LEU:O	1:A:105:GLY:N	1.96	0.97
1:A:81:LYS:HE2	1:A:297:PHE:HE1	1.20	0.96
1:A:278:SER:O	1:A:281:GLN:HG2	1.66	0.95
1:B:120:PHE:O	1:B:124:ASP:OD1	1.82	0.95
1:A:101:LEU:HB3	1:A:337:LEU:HB3	1.49	0.95
1:B:245:ILE:HD11	1:B:246:ILE:HG13	1.48	0.95
1:A:33:TYR:CZ	1:A:223:ASN:ND2	2.33	0.94
1:B:25:PRO:HB2	1:B:29:LEU:HB3	1.48	0.94
1:B:307:LEU:HD13	1:B:311:VAL:HG23	1.49	0.94
1:A:100:LEU:HD12	1:A:320:MSE:HG2	1.50	0.94
1:B:29:LEU:HD23	1:B:30:PHE:N	1.83	0.94
1:A:29:LEU:HD12	1:A:30:PHE:H	1.31	0.94
1:A:78:PHE:CE2	1:A:225:VAL:HG11	2.03	0.93
1:A:131:LEU:O	1:A:135:ALA:N	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ALA:O	1:B:244:VAL:HG23	1.68	0.93
1:A:240:LEU:O	1:A:244:VAL:HG23	1.69	0.92
1:A:156:LEU:HD23	1:A:157:ASN:H	1.28	0.92
1:A:224:LEU:CD1	1:A:228:PHE:HZ	1.82	0.92
1:B:117:ARG:HD2	1:B:267:LYS:HB3	1.51	0.92
1:B:89:LEU:O	1:B:93:THR:HG22	1.68	0.92
1:B:117:ARG:O	1:B:329:SER:HB2	1.68	0.92
1:A:100:LEU:CD1	1:A:320:MSE:HG2	2.00	0.91
1:A:21:LEU:O	1:A:23:HIS:CD2	2.24	0.90
1:A:78:PHE:HE2	1:A:225:VAL:HG13	1.11	0.89
1:A:131:LEU:N	1:A:131:LEU:HD12	1.87	0.89
1:A:224:LEU:HD22	1:A:228:PHE:HE2	1.33	0.89
1:A:132:LEU:CD2	1:A:317:VAL:HG13	2.03	0.88
1:A:30:PHE:CE1	1:A:224:LEU:HD22	2.08	0.88
1:B:99:ASN:HB2	1:B:252:ASN:HD21	1.35	0.87
1:A:167:ILE:HD11	1:A:288:PRO:HB2	1.57	0.87
1:A:81:LYS:CE	1:A:297:PHE:CE1	2.57	0.87
1:B:301:MSE:O	1:B:301:MSE:HG3	1.74	0.87
1:B:117:ARG:HA	1:B:117:ARG:NE	1.90	0.86
1:A:128:ASN:ND2	1:A:276:VAL:HG11	1.89	0.86
1:B:258:SER:O	1:B:261:ILE:HG13	1.76	0.86
1:A:29:LEU:HA	1:A:32:VAL:HG13	1.57	0.86
1:A:30:PHE:HB2	1:A:227:THR:CG2	2.04	0.85
1:A:33:TYR:CE2	1:A:223:ASN:HB3	2.10	0.85
1:A:97:LEU:O	1:A:100:LEU:O	1.94	0.85
1:B:94:GLY:HA3	1:B:244:VAL:HG22	1.56	0.85
1:A:21:LEU:O	1:A:23:HIS:NE2	2.10	0.85
1:A:81:LYS:CE	1:A:297:PHE:HE1	1.90	0.84
1:B:134:PHE:CD1	1:B:135:ALA:N	2.46	0.84
1:B:245:ILE:CD1	1:B:246:ILE:HG13	2.07	0.84
1:A:128:ASN:CG	1:A:276:VAL:HG11	1.98	0.84
1:B:287:ALA:HB3	1:B:288:PRO:HD3	1.59	0.83
1:B:296:PHE:CD2	1:B:297:PHE:CE1	2.62	0.83
1:B:99:ASN:ND2	1:B:279:THR:OG1	2.11	0.83
1:A:12:GLY:CA	1:A:36:THR:HG23	2.07	0.83
1:B:65:ALA:C	1:B:281:GLN:OE1	2.16	0.83
1:A:167:ILE:CD1	1:A:288:PRO:HB2	2.09	0.82
1:A:282:ILE:HG13	1:A:286:VAL:HG21	1.59	0.82
1:B:12:GLY:HA3	1:B:36:THR:CG2	2.05	0.82
1:A:30:PHE:CB	1:A:227:THR:HG21	2.10	0.82
1:B:296:PHE:HD2	1:B:297:PHE:CD1	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ALA:O	1:A:83:GLY:CA	2.28	0.82
1:B:135:ALA:O	1:B:139:ALA:HB3	1.80	0.81
1:B:252:ASN:O	1:B:256:HIS:HD2	1.63	0.81
1:B:117:ARG:H	1:B:329:SER:HB3	1.44	0.81
1:A:164:ILE:HD13	1:A:168:LEU:HD12	1.59	0.81
1:B:251:GLY:O	1:B:255:GLU:HG3	1.80	0.81
1:B:94:GLY:HA2	1:B:244:VAL:HG22	1.64	0.80
1:B:284:MSE:O	1:B:288:PRO:HG2	1.82	0.80
1:B:96:VAL:HG12	1:B:282:ILE:HD13	1.62	0.80
1:B:25:PRO:HB2	1:B:29:LEU:CB	2.10	0.80
1:B:307:LEU:CD1	1:B:311:VAL:HG23	2.11	0.80
1:A:141:VAL:HG22	1:A:310:LEU:HD21	1.64	0.80
1:B:249:ILE:HA	1:B:253:ALA:HB3	1.63	0.80
1:A:78:PHE:CZ	1:A:225:VAL:CG1	2.45	0.80
1:A:132:LEU:HD21	1:A:317:VAL:HG13	1.63	0.79
1:A:280:LEU:O	1:A:284:MSE:HG3	1.82	0.79
1:A:29:LEU:HA	1:A:32:VAL:HG12	1.63	0.79
1:B:131:LEU:HD13	1:B:280:LEU:HD22	1.64	0.79
1:A:12:GLY:HA3	1:A:36:THR:CG2	2.07	0.79
1:B:30:PHE:HD1	1:B:31:ALA:N	1.80	0.79
1:B:68:GLY:O	1:B:255:GLU:OE2	2.02	0.78
1:B:99:ASN:CB	1:B:252:ASN:ND2	2.46	0.78
1:A:311:VAL:O	1:A:315:SER:OG	2.02	0.78
1:B:24:TRP:N	1:B:25:PRO:CD	2.41	0.78
1:B:96:VAL:HG12	1:B:282:ILE:CG2	2.14	0.77
1:A:237:TRP:HD1	1:A:237:TRP:H	1.32	0.77
1:A:30:PHE:HE1	1:A:228:PHE:CZ	1.97	0.77
1:A:282:ILE:CA	1:A:286:VAL:CG2	2.41	0.77
1:B:103:VAL:HB	1:B:260:ILE:HD11	1.66	0.77
1:A:79:ALA:O	1:A:83:GLY:HA2	1.84	0.77
1:A:29:LEU:O	1:A:32:VAL:HG13	1.85	0.76
1:A:153:ALA:O	1:A:156:LEU:HD21	1.85	0.76
1:A:131:LEU:CD1	1:A:131:LEU:H	1.84	0.76
1:A:99:ASN:O	1:A:103:VAL:HG12	1.86	0.76
1:B:273:GLU:O	1:B:277:GLY:N	2.17	0.76
1:A:164:ILE:HD13	1:A:168:LEU:CG	2.16	0.75
1:B:134:PHE:CE1	1:B:284:MSE:HE1	2.21	0.75
1:B:30:PHE:C	1:B:30:PHE:CD1	2.60	0.75
1:A:138:VAL:HG12	1:A:139:ALA:N	2.01	0.75
1:B:330:ASN:HB2	1:B:333:GLU:CG	2.16	0.75
1:A:128:ASN:OD1	1:A:276:VAL:HG11	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:PHE:HD2	1:B:297:PHE:N	1.85	0.75
1:B:136:ILE:HG12	1:B:313:MSE:HE2	1.69	0.75
1:A:100:LEU:H	1:A:100:LEU:HD22	1.50	0.75
1:A:101:LEU:HD23	1:A:337:LEU:O	1.87	0.74
1:A:30:PHE:CD1	1:A:228:PHE:CE2	2.64	0.74
1:B:30:PHE:CD1	1:B:31:ALA:N	2.55	0.74
1:A:264:PHE:HD1	1:A:265:LYS:N	1.86	0.74
1:A:153:ALA:O	1:A:156:LEU:HD22	1.87	0.74
1:A:237:TRP:HB2	1:A:238:SER:HG	1.50	0.74
1:B:241:PHE:CE1	1:B:245:ILE:HG12	2.22	0.74
1:B:96:VAL:CG2	1:B:313:MSE:HE3	2.08	0.74
1:A:224:LEU:HD22	1:A:228:PHE:CZ	2.23	0.74
1:A:101:LEU:CD2	1:A:340:ALA:HB3	2.18	0.73
1:A:29:LEU:HD12	1:A:30:PHE:N	2.02	0.73
1:B:228:PHE:HA	1:B:231:VAL:HG23	1.70	0.73
1:A:100:LEU:HD12	1:A:320:MSE:CG	2.18	0.73
1:B:257:ALA:HA	1:B:260:ILE:CD1	2.18	0.73
1:A:30:PHE:CE1	1:A:224:LEU:CD2	2.71	0.73
1:B:330:ASN:HB2	1:B:333:GLU:HG3	1.71	0.73
1:A:81:LYS:HG2	1:A:297:PHE:CE1	2.24	0.72
1:A:330:ASN:H	1:A:333:GLU:HB2	1.54	0.72
1:A:125:ALA:O	1:A:129:SER:OG	2.07	0.72
1:A:139:ALA:O	1:A:143:PRO:HG2	1.89	0.72
1:A:67:PHE:HA	1:A:70:ALA:HB2	1.71	0.72
1:A:30:PHE:CD1	1:A:224:LEU:CD2	2.73	0.71
1:A:100:LEU:CD1	1:A:320:MSE:CG	2.68	0.71
1:B:117:ARG:HB2	1:B:329:SER:OG	1.90	0.71
1:B:133:ILE:HD11	1:B:137:ILE:CD1	2.15	0.71
1:B:99:ASN:HB2	1:B:252:ASN:HD22	1.52	0.71
1:B:307:LEU:CD1	1:B:311:VAL:CG2	2.68	0.71
1:A:30:PHE:CE1	1:A:228:PHE:CD2	2.75	0.71
1:A:93:THR:O	1:A:97:LEU:HD12	1.90	0.71
1:A:54:ILE:HD11	1:A:202:SER:HB3	1.72	0.71
1:B:133:ILE:HD13	1:B:137:ILE:HB	1.72	0.71
1:B:285:PHE:O	1:B:289:VAL:HG12	1.89	0.71
1:B:26:SER:O	1:B:29:LEU:HD22	1.89	0.71
1:A:26:SER:O	1:A:29:LEU:HD11	1.87	0.71
1:A:288:PRO:O	1:A:292:ILE:HG12	1.90	0.71
1:A:30:PHE:CD1	1:A:224:LEU:HD22	2.26	0.71
1:B:279:THR:O	1:B:282:ILE:HG22	1.91	0.71
1:A:138:VAL:CG1	1:A:139:ALA:N	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:N	1:A:142:ILE:HD13	2.05	0.71
1:B:282:ILE:HA	1:B:286:VAL:CG2	2.21	0.71
1:B:117:ARG:H	1:B:329:SER:CB	2.03	0.70
1:B:118:GLN:HB2	1:B:327:GLY:HA2	1.73	0.70
1:A:156:LEU:CD2	1:A:157:ASN:ND2	2.55	0.70
1:B:89:LEU:O	1:B:93:THR:CG2	2.40	0.70
1:A:29:LEU:CA	1:A:32:VAL:CG1	2.66	0.70
1:A:264:PHE:CD1	1:A:265:LYS:N	2.59	0.70
1:B:244:VAL:HG12	1:B:245:ILE:N	2.07	0.70
1:B:100:LEU:HG	1:B:320:MSE:HG3	1.72	0.70
1:A:83:GLY:HA2	1:A:84:LEU:CB	2.20	0.69
1:A:69:ASN:HD21	1:A:281:GLN:CD	1.87	0.69
1:B:29:LEU:HD23	1:B:30:PHE:H	1.55	0.69
1:B:282:ILE:HA	1:B:286:VAL:HG23	1.74	0.69
1:A:78:PHE:CD2	1:A:225:VAL:HG11	2.28	0.69
1:A:65:ALA:HA	1:A:281:GLN:NE2	2.08	0.69
1:A:73:LEU:O	1:A:77:MSE:HG2	1.92	0.69
1:B:241:PHE:O	1:B:245:ILE:HG13	1.93	0.69
1:B:85:THR:OG1	1:B:301:MSE:HB3	1.91	0.69
1:A:134:PHE:O	1:A:138:VAL:HB	1.93	0.69
1:B:25:PRO:CB	1:B:29:LEU:HB3	2.23	0.69
1:A:14:PRO:O	1:A:18:ILE:HG13	1.93	0.68
1:A:83:GLY:HA2	1:A:84:LEU:HB2	1.75	0.68
1:B:296:PHE:HD2	1:B:297:PHE:H	1.40	0.68
1:B:120:PHE:CE1	1:B:123:HIS:HB3	2.29	0.68
1:A:237:TRP:CD1	1:A:237:TRP:N	2.62	0.67
1:B:124:ASP:O	1:B:128:ASN:HB2	1.94	0.67
1:B:244:VAL:CG1	1:B:245:ILE:N	2.57	0.67
1:A:81:LYS:CD	1:A:297:PHE:CE1	2.78	0.67
1:B:251:GLY:C	1:B:255:GLU:OE1	2.33	0.67
1:A:137:ILE:O	1:A:141:VAL:HB	1.95	0.67
1:A:150:MSE:CE	1:A:155:LYS:HA	2.25	0.67
1:B:96:VAL:CG1	1:B:282:ILE:HD13	2.25	0.66
1:A:150:MSE:H	1:A:151:GLY:HA2	1.60	0.66
1:A:30:PHE:CD1	1:A:227:THR:HG21	2.31	0.66
1:A:129:SER:HB3	1:A:321:ILE:HD11	1.76	0.66
1:A:85:THR:OG1	1:A:301:MSE:HB2	1.93	0.66
1:A:150:MSE:HE1	1:A:155:LYS:HA	1.76	0.66
1:A:164:ILE:HD12	1:A:168:LEU:HD11	1.68	0.66
1:A:30:PHE:HE1	1:A:224:LEU:HD22	1.57	0.66
1:A:264:PHE:C	1:A:264:PHE:CD1	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:HA	1:A:103:VAL:HG12	1.77	0.66
1:B:241:PHE:CD1	1:B:245:ILE:HG12	2.31	0.65
1:A:298:PRO:HB3	1:B:82:GLU:HA	1.79	0.65
1:A:287:ALA:HB3	1:A:288:PRO:HD3	1.79	0.65
1:B:164:ILE:O	1:B:168:LEU:HG	1.96	0.65
1:A:134:PHE:CD2	1:A:135:ALA:N	2.64	0.65
1:B:117:ARG:HA	1:B:117:ARG:HE	1.62	0.65
1:B:256:HIS:CE1	1:B:278:SER:CB	2.80	0.65
1:B:96:VAL:HG21	1:B:313:MSE:CE	2.10	0.64
1:A:78:PHE:HE2	1:A:225:VAL:CG1	1.80	0.64
1:B:88:VAL:O	1:B:92:LEU:HD23	1.98	0.64
1:B:259:ALA:HA	1:B:262:MSE:HB3	1.79	0.64
1:A:29:LEU:CA	1:A:32:VAL:HG13	2.24	0.64
1:B:257:ALA:HA	1:B:260:ILE:HD13	1.78	0.64
1:A:101:LEU:HD21	1:A:340:ALA:HB3	1.80	0.64
1:A:113:LEU:HD12	1:A:114:LYS:H	1.62	0.64
1:A:28:VAL:O	1:A:31:ALA:HB3	1.99	0.63
1:B:129:SER:O	1:B:130:GLY:C	2.34	0.63
1:A:142:ILE:HB	1:A:143:PRO:HD3	1.80	0.63
1:A:128:ASN:HD21	1:A:276:VAL:HG11	1.62	0.63
1:A:231:VAL:O	1:A:235:PHE:O	2.16	0.63
1:B:258:SER:O	1:B:261:ILE:CG1	2.45	0.63
1:B:244:VAL:HG12	1:B:245:ILE:H	1.63	0.63
1:B:120:PHE:CZ	1:B:123:HIS:HB3	2.34	0.62
1:B:134:PHE:HA	1:B:138:VAL:HG23	1.80	0.62
1:B:303:LEU:CD2	1:B:305:PHE:HE2	2.13	0.62
1:A:113:LEU:HD12	1:A:114:LYS:N	2.15	0.62
1:A:134:PHE:CD2	1:A:134:PHE:C	2.73	0.62
1:A:128:ASN:C	1:A:128:ASN:HD22	2.03	0.62
1:A:132:LEU:HD21	1:A:317:VAL:HG22	1.80	0.62
1:B:281:GLN:O	1:B:286:VAL:HG23	2.00	0.61
1:B:101:LEU:HD13	1:B:316:ALA:HB1	1.81	0.61
1:B:128:ASN:O	1:B:132:LEU:HB2	1.99	0.61
1:B:285:PHE:O	1:B:289:VAL:CG1	2.48	0.61
1:A:101:LEU:CD2	1:A:337:LEU:O	2.48	0.61
1:A:225:VAL:HG23	1:A:226:HIS:N	2.15	0.61
1:B:5:PHE:HD1	1:B:39:ALA:HA	1.65	0.61
1:A:130:GLY:O	1:A:134:PHE:HB3	2.00	0.60
1:B:287:ALA:HB3	1:B:288:PRO:CD	2.31	0.60
1:B:296:PHE:CD2	1:B:297:PHE:HD1	2.13	0.60
1:A:70:ALA:O	1:A:74:ILE:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:HG2	1:A:297:PHE:CD1	2.36	0.60
1:B:296:PHE:CE2	1:B:297:PHE:CD1	2.76	0.60
1:A:164:ILE:HD13	1:A:168:LEU:HG	1.83	0.59
1:B:256:HIS:CE1	1:B:278:SER:HB2	2.36	0.59
1:A:274:ILE:O	1:A:278:SER:HB3	2.02	0.59
1:B:256:HIS:CE1	1:B:278:SER:HB3	2.37	0.59
1:B:262:MSE:HE3	1:B:265:LYS:HB3	1.85	0.59
1:B:24:TRP:N	1:B:25:PRO:HD3	2.08	0.58
1:B:91:SER:O	1:B:95:SER:OG	2.13	0.58
1:B:92:LEU:O	1:B:96:VAL:HG13	2.04	0.58
1:B:94:GLY:CA	1:B:244:VAL:CG2	2.73	0.58
1:A:98:GLY:O	1:A:102:LEU:HB3	2.03	0.58
1:A:28:VAL:O	1:A:32:VAL:HG12	2.04	0.58
1:B:328:ASP:OD2	1:B:328:ASP:N	2.37	0.58
1:B:94:GLY:HA3	1:B:244:VAL:CG2	2.30	0.58
1:A:133:ILE:O	1:A:137:ILE:HB	2.04	0.58
1:B:262:MSE:HG3	1:B:262:MSE:O	2.02	0.57
1:A:268:MSE:HG2	1:A:271:ALA:HB3	1.87	0.57
1:B:301:MSE:O	1:B:301:MSE:CG	2.51	0.57
1:B:12:GLY:CA	1:B:36:THR:HG21	2.13	0.57
1:B:296:PHE:CD2	1:B:297:PHE:N	2.70	0.57
1:B:25:PRO:CB	1:B:29:LEU:CB	2.81	0.57
1:B:166:MSE:HE2	1:B:284:MSE:HG2	1.87	0.56
1:B:236:GLY:C	1:B:237:TRP:CD2	2.78	0.56
1:A:164:ILE:CD1	1:A:168:LEU:HD12	2.21	0.56
1:A:34:CYS:SG	1:A:35:VAL:N	2.79	0.56
1:B:134:PHE:HD1	1:B:135:ALA:N	2.00	0.56
1:A:225:VAL:CG2	1:A:226:HIS:N	2.68	0.56
1:A:120:PHE:CZ	1:A:269:ASP:HB2	2.41	0.56
1:B:144:GLU:OE1	1:B:304:VAL:HB	2.06	0.55
1:B:24:TRP:H	1:B:25:PRO:HD2	1.65	0.55
1:B:26:SER:O	1:B:29:LEU:CD2	2.53	0.55
1:B:304:VAL:HG23	1:B:304:VAL:O	2.06	0.55
1:A:81:LYS:CG	1:A:297:PHE:CE1	2.89	0.55
1:B:303:LEU:CD2	1:B:305:PHE:CE2	2.89	0.55
1:A:156:LEU:CD2	1:A:157:ASN:H	2.11	0.55
1:A:307:LEU:N	1:A:308:PRO:HD2	2.21	0.55
1:B:132:LEU:HD13	1:B:317:VAL:HG13	1.88	0.55
1:B:225:VAL:HA	1:B:228:PHE:CE2	2.41	0.55
1:A:158:LEU:O	1:A:162:ILE:HG13	2.06	0.55
1:A:98:GLY:C	1:A:100:LEU:O	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ILE:CG2	1:B:283:ALA:N	2.69	0.55
1:A:13:VAL:CG1	1:A:14:PRO:HD3	2.37	0.55
1:A:138:VAL:O	1:A:142:ILE:HG12	2.07	0.55
1:A:99:ASN:CA	1:A:103:VAL:HG12	2.37	0.54
1:B:85:THR:OG1	1:B:301:MSE:CB	2.55	0.54
1:A:142:ILE:H	1:A:142:ILE:HD13	1.72	0.54
1:A:224:LEU:O	1:A:228:PHE:CE2	2.60	0.54
1:A:242:ILE:HA	1:A:246:ILE:HD12	1.88	0.54
1:B:228:PHE:HA	1:B:231:VAL:CG2	2.36	0.54
1:A:59:ILE:H	1:A:59:ILE:HD13	1.73	0.54
1:B:266:ASN:HD22	1:B:270:ILE:HG22	1.72	0.54
1:B:69:ASN:HB2	1:B:281:GLN:NE2	2.23	0.54
1:A:134:PHE:HD2	1:A:135:ALA:N	2.07	0.53
1:B:136:ILE:CG1	1:B:313:MSE:HE2	2.38	0.53
1:B:266:ASN:O	1:B:268:MSE:HA	2.08	0.53
1:A:282:ILE:C	1:A:286:VAL:HG23	2.26	0.53
1:B:117:ARG:C	1:B:329:SER:HB2	2.27	0.53
1:A:171:VAL:O	1:A:175:TYR:HB2	2.08	0.53
1:B:228:PHE:CA	1:B:231:VAL:HG23	2.36	0.53
1:B:262:MSE:HE1	1:B:265:LYS:HD2	1.91	0.53
1:B:101:LEU:HD23	1:B:341:TYR:CA	2.39	0.53
1:B:284:MSE:O	1:B:288:PRO:CG	2.54	0.53
1:A:100:LEU:HD11	1:A:320:MSE:CG	2.37	0.53
1:B:162:ILE:HD11	1:B:303:LEU:HD13	1.90	0.53
1:B:237:TRP:N	1:B:237:TRP:CE3	2.76	0.53
1:A:135:ALA:O	1:A:139:ALA:CB	2.56	0.53
1:A:140:PHE:HD1	1:A:305:PHE:CE2	2.27	0.53
1:A:119:GLU:O	1:A:328:ASP:HA	2.09	0.53
1:A:156:LEU:HD23	1:A:157:ASN:ND2	2.22	0.52
1:A:224:LEU:CG	1:A:228:PHE:HZ	2.22	0.52
1:A:95:SER:HB3	1:A:252:ASN:ND2	2.23	0.52
1:B:15:LEU:HA	1:B:18:ILE:HD12	1.90	0.52
1:A:237:TRP:HD1	1:A:237:TRP:N	2.01	0.52
1:A:83:GLY:CA	1:A:84:LEU:HB2	2.39	0.52
1:A:41:ALA:HA	1:A:44:MSE:HB2	1.92	0.52
1:B:4:ILE:HD12	1:B:4:ILE:H	1.74	0.52
1:B:298:PRO:HA	1:B:300:SER:OG	2.09	0.52
1:A:93:THR:HG22	1:A:97:LEU:CD1	2.39	0.52
1:B:137:ILE:O	1:B:141:VAL:HB	2.09	0.52
1:A:102:LEU:O	1:A:106:LEU:HB2	2.10	0.52
1:A:30:PHE:CG	1:A:227:THR:HG21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:SER:H	1:A:241:PHE:HB3	1.74	0.52
1:B:237:TRP:N	1:B:237:TRP:CD2	2.77	0.52
1:A:122:ILE:HG22	1:A:126:ARG:HH21	1.74	0.52
1:A:33:TYR:CE2	1:A:223:ASN:CB	2.90	0.51
1:B:234:GLN:OE1	1:B:234:GLN:HA	2.09	0.51
1:B:143:PRO:O	1:B:147:SER:HB2	2.10	0.51
1:A:156:LEU:HD23	1:A:156:LEU:C	2.22	0.51
1:B:249:ILE:HA	1:B:253:ALA:CB	2.37	0.51
1:B:142:ILE:O	1:B:146:PHE:HB2	2.11	0.51
1:B:263:ALA:O	1:B:266:ASN:O	2.29	0.51
1:A:138:VAL:HG12	1:A:139:ALA:H	1.72	0.51
1:A:29:LEU:CD1	1:A:30:PHE:N	2.73	0.51
1:A:163:SER:HA	1:A:166:MSE:HE3	1.93	0.50
1:A:132:LEU:HD23	1:A:132:LEU:C	2.31	0.50
1:A:76:SER:HB3	1:A:88:VAL:HG13	1.93	0.50
1:B:227:THR:O	1:B:231:VAL:HG23	2.11	0.50
1:A:79:ALA:O	1:A:83:GLY:N	2.44	0.50
1:A:167:ILE:HD12	1:A:288:PRO:HB2	1.92	0.50
1:B:299:THR:O	1:B:300:SER:CB	2.59	0.50
1:A:224:LEU:HB3	1:A:228:PHE:CZ	2.47	0.50
1:B:106:LEU:HD23	1:B:260:ILE:HG21	1.93	0.50
1:A:99:ASN:C	1:A:103:VAL:HG12	2.32	0.49
1:A:162:ILE:HG22	1:A:166:MSE:HE2	1.94	0.49
1:A:159:SER:OG	1:A:291:VAL:HG11	2.13	0.49
1:B:101:LEU:HD23	1:B:341:TYR:HB2	1.93	0.49
1:B:134:PHE:CD1	1:B:134:PHE:C	2.85	0.49
1:B:288:PRO:O	1:B:292:ILE:HG12	2.13	0.49
1:A:129:SER:CB	1:A:321:ILE:HD11	2.43	0.49
1:A:100:LEU:HD12	1:A:320:MSE:SE	2.62	0.49
1:B:241:PHE:CZ	1:B:245:ILE:HG12	2.47	0.49
1:B:134:PHE:CD1	1:B:135:ALA:CA	2.96	0.49
1:B:99:ASN:CB	1:B:252:ASN:HD22	2.19	0.49
1:A:156:LEU:CD2	1:A:157:ASN:N	2.56	0.49
1:A:224:LEU:CD2	1:A:228:PHE:CZ	2.96	0.49
1:B:216:VAL:O	1:B:220:ILE:HG13	2.13	0.49
1:B:282:ILE:HG23	1:B:283:ALA:N	2.26	0.49
1:B:300:SER:O	1:B:301:MSE:C	2.51	0.49
1:B:121:ASN:ND2	1:B:326:ASP:HA	2.27	0.49
1:A:150:MSE:HE3	1:A:155:LYS:N	2.28	0.48
1:A:123:HIS:O	1:A:127:HIS:CD2	2.66	0.48
1:A:29:LEU:C	1:A:32:VAL:HG13	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:ND2	1:A:157:ASN:H	2.11	0.48
1:B:133:ILE:HD13	1:B:137:ILE:CB	2.43	0.48
1:A:101:LEU:N	1:A:101:LEU:CD1	2.76	0.48
1:B:118:GLN:CB	1:B:327:GLY:HA2	2.41	0.48
1:A:78:PHE:CZ	1:A:221:SER:O	2.66	0.48
1:B:95:SER:HB2	1:B:282:ILE:HD11	1.95	0.48
1:B:29:LEU:HD21	1:B:227:THR:HG21	1.96	0.48
1:B:84:LEU:HD12	1:B:87:ILE:N	2.29	0.48
1:A:128:ASN:O	1:A:132:LEU:HB2	2.13	0.48
1:A:147:SER:HA	1:A:150:MSE:HE2	1.96	0.48
1:A:81:LYS:HD3	1:A:297:PHE:CZ	2.49	0.48
1:B:245:ILE:HD11	1:B:246:ILE:CG1	2.32	0.48
1:B:117:ARG:HB2	1:B:329:SER:CB	2.43	0.48
1:A:150:MSE:N	1:A:151:GLY:HA2	2.23	0.48
1:A:22:MSE:C	1:A:23:HIS:CD2	2.87	0.48
1:A:237:TRP:HB2	1:A:238:SER:CB	2.42	0.48
1:A:332:PHE:O	1:A:336:THR:OG1	2.32	0.48
1:B:133:ILE:O	1:B:137:ILE:HB	2.14	0.48
1:B:117:ARG:CA	1:B:329:SER:HB2	2.44	0.48
1:B:243:GLY:O	1:B:247:VAL:HB	2.14	0.47
1:B:338:LEU:O	1:B:342:VAL:HG23	2.13	0.47
1:A:128:ASN:OD1	1:A:276:VAL:CG1	2.60	0.47
1:A:280:LEU:HD22	1:A:284:MSE:HE2	1.95	0.47
1:B:259:ALA:HB2	1:B:274:ILE:HG21	1.96	0.47
1:A:93:THR:HG22	1:A:97:LEU:HD11	1.95	0.47
1:B:259:ALA:O	1:B:262:MSE:HB3	2.15	0.47
1:A:131:LEU:HA	1:A:134:PHE:HB3	1.96	0.47
1:A:164:ILE:O	1:A:168:LEU:HG	2.14	0.47
1:A:224:LEU:O	1:A:227:THR:HB	2.15	0.47
1:A:156:LEU:H	1:A:156:LEU:HD22	1.80	0.47
1:B:223:ASN:O	1:B:227:THR:HG23	2.13	0.47
1:B:84:LEU:HD12	1:B:87:ILE:H	1.78	0.47
1:A:142:ILE:HB	1:A:143:PRO:CD	2.44	0.47
1:A:282:ILE:HG22	1:A:283:ALA:N	2.29	0.47
1:A:128:ASN:C	1:A:128:ASN:ND2	2.68	0.47
1:A:152:ASN:HA	1:A:155:LYS:HD3	1.96	0.47
1:A:164:ILE:HD12	1:A:168:LEU:CD1	2.30	0.47
1:A:139:ALA:O	1:A:143:PRO:CG	2.60	0.47
1:A:224:LEU:CG	1:A:228:PHE:CZ	2.97	0.47
1:A:101:LEU:N	1:A:101:LEU:HD12	2.30	0.47
1:A:95:SER:CB	1:A:252:ASN:HD22	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:O	1:A:228:PHE:CD2	2.68	0.46
1:A:95:SER:CB	1:A:252:ASN:ND2	2.78	0.46
1:B:117:ARG:N	1:B:329:SER:CB	2.76	0.46
1:A:68:GLY:O	1:A:255:GLU:CD	2.54	0.46
1:B:245:ILE:HD12	1:B:245:ILE:C	2.35	0.46
1:B:129:SER:HB3	1:B:321:ILE:HG12	1.98	0.46
1:A:13:VAL:HG13	1:A:14:PRO:HD3	1.96	0.46
1:B:141:VAL:HG22	1:B:310:LEU:HD21	1.98	0.46
1:B:101:LEU:HD23	1:B:341:TYR:CB	2.45	0.46
1:B:124:ASP:N	1:B:124:ASP:OD1	2.40	0.46
1:B:217:VAL:HA	1:B:220:ILE:HD12	1.98	0.46
1:B:307:LEU:HD12	1:B:311:VAL:CG2	2.46	0.46
1:A:224:LEU:CB	1:A:228:PHE:CZ	2.99	0.46
1:A:18:ILE:HG22	1:A:22:MSE:SE	2.65	0.46
1:B:139:ALA:CB	1:B:166:MSE:HE3	2.46	0.46
1:B:252:ASN:O	1:B:256:HIS:CD2	2.55	0.46
1:A:95:SER:HB3	1:A:282:ILE:HG12	1.98	0.45
1:A:30:PHE:CD1	1:A:227:THR:CG2	2.98	0.45
1:B:287:ALA:CB	1:B:288:PRO:HD3	2.39	0.45
1:B:133:ILE:HD13	1:B:137:ILE:HD12	1.89	0.45
1:B:31:ALA:O	1:B:35:VAL:HG23	2.17	0.45
1:B:251:GLY:O	1:B:255:GLU:CG	2.58	0.45
1:A:297:PHE:CD2	1:A:298:PRO:HD2	2.52	0.45
1:A:130:GLY:O	1:A:134:PHE:CB	2.65	0.45
1:A:147:SER:HB2	1:A:155:LYS:HG2	1.98	0.45
1:B:120:PHE:C	1:B:124:ASP:OD1	2.51	0.45
1:A:81:LYS:HE2	1:A:297:PHE:CD1	2.45	0.45
1:B:330:ASN:HB2	1:B:333:GLU:CB	2.46	0.45
1:A:90:ALA:HB1	1:A:244:VAL:HG22	1.99	0.44
1:A:99:ASN:ND2	1:A:279:THR:OG1	2.34	0.44
1:B:236:GLY:C	1:B:237:TRP:CG	2.90	0.44
1:A:99:ASN:C	1:A:100:LEU:O	2.51	0.44
1:B:294:SER:OG	1:B:300:SER:HA	2.17	0.44
1:A:99:ASN:HA	1:A:103:VAL:CG1	2.45	0.44
1:B:122:ILE:HG23	1:B:123:HIS:N	2.31	0.44
1:B:30:PHE:HA	1:B:33:TYR:CD2	2.53	0.44
1:A:263:ALA:O	1:A:264:PHE:HB3	2.16	0.44
1:B:163:SER:OG	1:B:288:PRO:HB3	2.17	0.44
1:B:101:LEU:HD23	1:B:341:TYR:HA	1.99	0.44
1:B:24:TRP:N	1:B:25:PRO:HD2	2.28	0.44
1:A:37:ILE:HA	1:A:40:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HG13	1:B:163:SER:N	2.31	0.44
1:A:135:ALA:O	1:A:139:ALA:HB3	2.18	0.44
1:A:96:VAL:CG2	1:A:97:LEU:N	2.80	0.44
1:B:96:VAL:CG1	1:B:282:ILE:HG21	2.26	0.44
1:A:142:ILE:N	1:A:142:ILE:CD1	2.75	0.44
1:B:134:PHE:CZ	1:B:169:LEU:HD23	2.53	0.44
1:B:158:LEU:O	1:B:162:ILE:HG23	2.17	0.44
1:B:257:ALA:HA	1:B:260:ILE:HD12	1.97	0.43
1:B:326:ASP:HB3	1:B:327:GLY:H	1.60	0.43
1:A:162:ILE:O	1:A:165:ILE:HG13	2.18	0.43
1:B:330:ASN:HD22	1:B:333:GLU:CG	2.31	0.43
1:A:128:ASN:O	1:A:132:LEU:CB	2.66	0.43
1:B:5:PHE:CD1	1:B:39:ALA:HA	2.50	0.43
1:B:167:ILE:O	1:B:171:VAL:HG22	2.19	0.43
1:A:256:HIS:CE1	1:A:278:SER:HB2	2.54	0.43
1:B:29:LEU:HD21	1:B:227:THR:CG2	2.47	0.43
1:A:84:LEU:HD22	1:A:87:ILE:HG13	2.00	0.43
1:B:307:LEU:HD22	1:B:307:LEU:HA	1.76	0.43
1:A:137:ILE:HG22	1:A:138:VAL:N	2.34	0.42
1:A:205:VAL:HA	1:A:208:ILE:HG22	2.01	0.42
1:A:25:PRO:O	1:A:29:LEU:HG	2.20	0.42
1:B:244:VAL:HG12	1:B:245:ILE:HG23	2.01	0.42
1:B:262:MSE:HG2	1:B:270:ILE:HG23	2.00	0.42
1:B:286:VAL:O	1:B:290:LEU:HB2	2.18	0.42
1:A:30:PHE:CE1	1:A:224:LEU:HD21	2.53	0.42
1:A:289:VAL:CG2	1:A:290:LEU:N	2.83	0.42
1:A:97:LEU:O	1:A:100:LEU:C	2.56	0.42
1:A:101:LEU:H	1:A:101:LEU:CD1	2.33	0.42
1:A:136:ILE:HD13	1:A:140:PHE:CE2	2.54	0.42
1:B:100:LEU:HD23	1:B:100:LEU:C	2.39	0.42
1:A:100:LEU:CD2	1:A:100:LEU:H	2.24	0.42
1:A:150:MSE:HB3	1:A:154:SER:HB2	2.01	0.42
1:B:245:ILE:HG13	1:B:246:ILE:N	2.35	0.42
1:A:148:VAL:HG13	1:A:149:GLY:N	2.34	0.42
1:B:164:ILE:HG13	1:B:165:ILE:N	2.35	0.42
1:A:282:ILE:CA	1:A:286:VAL:HG21	2.33	0.42
1:A:29:LEU:O	1:A:33:TYR:N	2.31	0.42
1:B:99:ASN:CB	1:B:252:ASN:HD21	2.14	0.42
1:A:148:VAL:HG13	1:A:149:GLY:H	1.84	0.42
1:B:99:ASN:CG	1:B:100:LEU:N	2.73	0.42
1:B:259:ALA:HA	1:B:262:MSE:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASN:HB2	1:B:281:GLN:HE22	1.83	0.42
1:B:134:PHE:HA	1:B:138:VAL:CG2	2.47	0.41
1:B:242:ILE:O	1:B:246:ILE:HB	2.20	0.41
1:A:292:ILE:O	1:A:295:ILE:HG12	2.21	0.41
1:A:26:SER:HA	1:A:29:LEU:HD11	2.03	0.41
1:B:152:ASN:HD21	1:B:299:THR:HG23	1.86	0.41
1:B:298:PRO:HA	1:B:299:THR:C	2.41	0.41
1:A:129:SER:HB3	1:A:321:ILE:CD1	2.46	0.41
1:A:156:LEU:N	1:A:156:LEU:HD22	2.34	0.41
1:B:120:PHE:CZ	1:B:123:HIS:CD2	3.09	0.41
1:B:133:ILE:CD1	1:B:137:ILE:CD1	2.76	0.41
1:A:249:ILE:HG22	1:A:250:VAL:N	2.36	0.41
1:B:65:ALA:O	1:B:281:GLN:CD	2.54	0.41
1:A:33:TYR:O	1:A:37:ILE:HG13	2.20	0.41
1:B:10:ALA:O	1:B:14:PRO:HG2	2.20	0.41
1:B:242:ILE:O	1:B:247:VAL:HG23	2.21	0.41
1:A:156:LEU:HD21	1:A:157:ASN:ND2	2.33	0.41
1:B:264:PHE:CD1	1:B:267:LYS:HE3	2.55	0.41
1:B:96:VAL:CG1	1:B:282:ILE:CG2	2.94	0.41
1:B:330:ASN:CB	1:B:333:GLU:HG3	2.47	0.41
1:A:132:LEU:HD21	1:A:317:VAL:CG1	2.41	0.41
1:A:166:MSE:HE3	1:A:288:PRO:HG3	2.03	0.41
1:B:124:ASP:O	1:B:128:ASN:CB	2.65	0.41
1:B:99:ASN:HA	1:B:103:VAL:HG13	2.03	0.41
1:A:78:PHE:HE2	1:A:225:VAL:CB	2.33	0.41
1:A:140:PHE:CD1	1:A:305:PHE:CZ	3.09	0.41
1:A:139:ALA:HB2	1:A:166:MSE:SE	2.71	0.41
1:A:174:LEU:HD22	1:A:177:LYS:HD3	2.03	0.41
1:B:13:VAL:HB	1:B:14:PRO:HD3	2.02	0.41
1:A:78:PHE:HE2	1:A:225:VAL:CG2	2.34	0.41
1:B:240:LEU:O	1:B:243:GLY:N	2.54	0.41
1:A:140:PHE:HD1	1:A:305:PHE:CZ	2.38	0.40
1:A:161:GLY:O	1:A:164:ILE:HG22	2.21	0.40
1:A:330:ASN:N	1:A:333:GLU:HB2	2.30	0.40
1:B:330:ASN:ND2	1:B:333:GLU:HG3	2.36	0.40
1:A:156:LEU:CD2	1:A:156:LEU:N	2.83	0.40
1:A:41:ALA:O	1:A:255:GLU:HA	2.22	0.40
1:A:268:MSE:HE3	1:A:268:MSE:HB3	2.00	0.40
1:A:314:VAL:O	1:A:318:LEU:HG	2.21	0.40
1:B:172:ALA:O	1:B:176:PHE:HB2	2.21	0.40
1:B:24:TRP:CD1	1:B:24:TRP:C	2.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ALA:HA	1:B:338:LEU:HB2	2.03	0.40
1:B:93:THR:O	1:B:96:VAL:HG22	2.22	0.40
1:A:285:PHE:O	1:A:286:VAL:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/351 (91%)	295 (92%)	24 (8%)	0	100	100
1	B	305/351 (87%)	286 (94%)	17 (6%)	2 (1%)	25	67
All	All	624/702 (89%)	581 (93%)	41 (7%)	2 (0%)	44	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	TRP
1	B	251	GLY

5.3.2 Protein sidechains [i](#)

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	259/267 (97%)	200 (77%)	59 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	247/267 (92%)	187 (76%)	60 (24%)	1	4
All	All	506/534 (95%)	387 (76%)	119 (24%)	1	4

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	22	MSE
1	A	24	TRP
1	A	28	VAL
1	A	29	LEU
1	A	32	VAL
1	A	35	VAL
1	A	36	THR
1	A	59	ILE
1	A	73	LEU
1	A	74	ILE
1	A	85	THR
1	A	91	SER
1	A	101	LEU
1	A	110	VAL
1	A	115	TYR
1	A	117	ARG
1	A	119	GLU
1	A	122	ILE
1	A	127	HIS
1	A	128	ASN
1	A	129	SER
1	A	131	LEU
1	A	134	PHE
1	A	137	ILE
1	A	138	VAL
1	A	142	ILE
1	A	144	GLU
1	A	150	MSE
1	A	156	LEU
1	A	157	ASN
1	A	159	SER
1	A	162	ILE
1	A	164	ILE
1	A	174	LEU
1	A	175	TYR

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Mol	Chain	Res	Type
1	A	177	LYS
1	A	224	LEU
1	A	237	TRP
1	A	239	GLU
1	A	249	ILE
1	A	264	PHE
1	A	268	MSE
1	A	278	SER
1	A	281	GLN
1	A	282	ILE
1	A	284	MSE
1	A	286	VAL
1	A	289	VAL
1	A	297	PHE
1	A	301	MSE
1	A	315	SER
1	A	320	MSE
1	A	326	ASP
1	A	329	SER
1	A	332	PHE
1	A	336	THR
1	A	343	ILE
1	A	350	LEU
1	B	7	ILE
1	B	9	VAL
1	B	24	TRP
1	B	28	VAL
1	B	29	LEU
1	B	30	PHE
1	B	69	ASN
1	B	77	MSE
1	B	82	GLU
1	B	84	LEU
1	B	93	THR
1	B	99	ASN
1	B	100	LEU
1	B	102	LEU
1	B	103	VAL
1	B	114	LYS
1	B	115	TYR
1	B	117	ARG
1	B	124	ASP

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Mol	Chain	Res	Type
1	B	127	HIS
1	B	129	SER
1	B	131	LEU
1	B	132	LEU
1	B	133	ILE
1	B	134	PHE
1	B	136	ILE
1	B	142	ILE
1	B	158	LEU
1	B	166	MSE
1	B	174	LEU
1	B	177	LYS
1	B	207	THR
1	B	224	LEU
1	B	229	HIS
1	B	231	VAL
1	B	233	GLU
1	B	237	TRP
1	B	244	VAL
1	B	245	ILE
1	B	264	PHE
1	B	268	MSE
1	B	281	GLN
1	B	289	VAL
1	B	290	LEU
1	B	296	PHE
1	B	300	SER
1	B	301	MSE
1	B	303	LEU
1	B	307	LEU
1	B	310	LEU
1	B	314	VAL
1	B	315	SER
1	B	319	LEU
1	B	320	MSE
1	B	326	ASP
1	B	328	ASP
1	B	329	SER
1	B	331	TRP
1	B	332	PHE
1	B	350	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	127	HIS
1	A	223	ASN
1	A	252	ASN
1	A	256	HIS
1	A	266	ASN
1	B	69	ASN
1	B	99	ASN
1	B	152	ASN
1	B	252	ASN
1	B	256	HIS
1	B	266	ASN
1	B	281	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	313/351 (89%)	-0.45	5 (1%)	72 44	50, 90, 131, 157	0
1	B	299/351 (85%)	-0.47	4 (1%)	77 51	47, 87, 123, 143	0
All	All	612/702 (87%)	-0.46	9 (1%)	74 47	47, 89, 126, 157	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	PHE	4.4
1	A	266	ASN	3.2
1	B	7	ILE	3.1
1	A	127	HIS	2.7
1	B	5	PHE	2.6
1	B	113	LEU	2.4
1	B	265	LYS	2.3
1	A	175	TYR	2.2
1	A	296	PHE	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.