Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:30 PM GMT

PDB ID	:	4LTO
Title	:	Bacterial sodium channel in high calcium, I222 space group
Authors	:	Shaya, D.; Findeisen, F.; Abderemane-Ali, F.; Arrigoni, C.; Wong, S.; Reddy Nurva, S.; Loussouarn, G.; Minor, D.L.
Deposited on	:	2013-07-23
Resolution	:	3.46 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

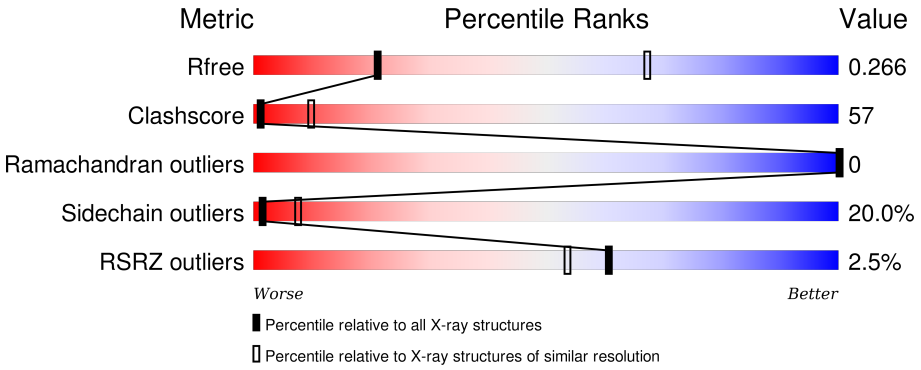
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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 <=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	152	2% 33% 43% 14% • 9%
1	B	152	3% 39% 41% 9% • 9%
1	C	152	% 38% 47% 6% 9%
1	D	152	3% 34% 46% 11% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4095 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1029	687	156	180	6			
1	B	138	Total	C	N	O	S	0	0	0
			1025	687	155	177	6			
1	C	138	Total	C	N	O	S	0	0	0
			1020	684	157	173	6			
1	D	138	Total	C	N	O	S	0	0	0
			1010	678	155	171	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	EXPRESSION TAG	UNP Q0ABW0
A	138	PRO	-	EXPRESSION TAG	UNP Q0ABW0
A	139	SER	-	EXPRESSION TAG	UNP Q0ABW0
A	140	SER	-	EXPRESSION TAG	UNP Q0ABW0
A	141	PRO	-	EXPRESSION TAG	UNP Q0ABW0
A	142	SER	-	EXPRESSION TAG	UNP Q0ABW0
B	137	GLY	-	EXPRESSION TAG	UNP Q0ABW0
B	138	PRO	-	EXPRESSION TAG	UNP Q0ABW0
B	139	SER	-	EXPRESSION TAG	UNP Q0ABW0
B	140	SER	-	EXPRESSION TAG	UNP Q0ABW0
B	141	PRO	-	EXPRESSION TAG	UNP Q0ABW0
B	142	SER	-	EXPRESSION TAG	UNP Q0ABW0
C	137	GLY	-	EXPRESSION TAG	UNP Q0ABW0
C	138	PRO	-	EXPRESSION TAG	UNP Q0ABW0
C	139	SER	-	EXPRESSION TAG	UNP Q0ABW0
C	140	SER	-	EXPRESSION TAG	UNP Q0ABW0
C	141	PRO	-	EXPRESSION TAG	UNP Q0ABW0
C	142	SER	-	EXPRESSION TAG	UNP Q0ABW0
D	137	GLY	-	EXPRESSION TAG	UNP Q0ABW0
D	138	PRO	-	EXPRESSION TAG	UNP Q0ABW0
D	139	SER	-	EXPRESSION TAG	UNP Q0ABW0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	140	SER	-	EXPRESSION TAG	UNP Q0ABW0
D	141	PRO	-	EXPRESSION TAG	UNP Q0ABW0
D	142	SER	-	EXPRESSION TAG	UNP Q0ABW0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Ca 3 3	0	0
2	A	2	Total Ca 2 2	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

- Molecule 4 is water.

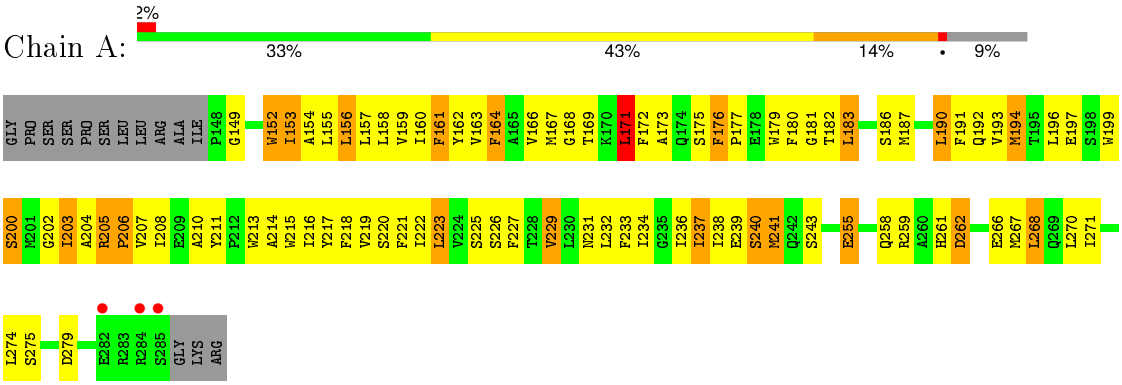
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

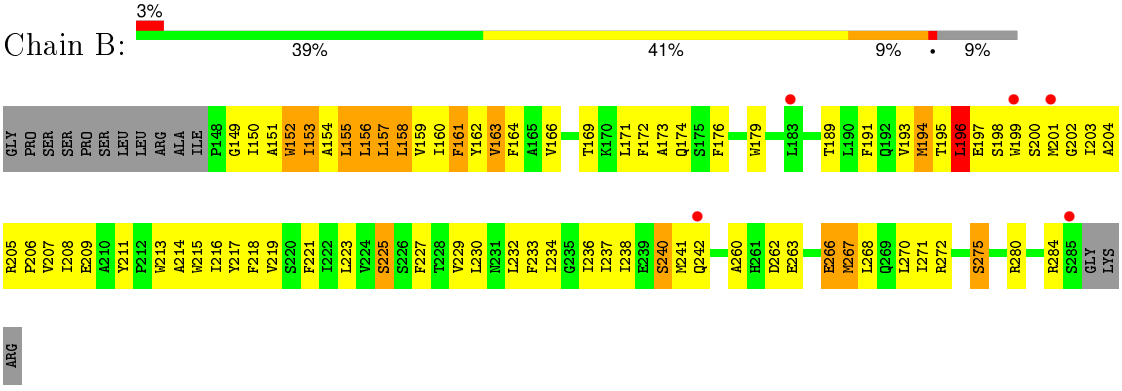
- Molecule 1: Ion transport protein

Chain A:



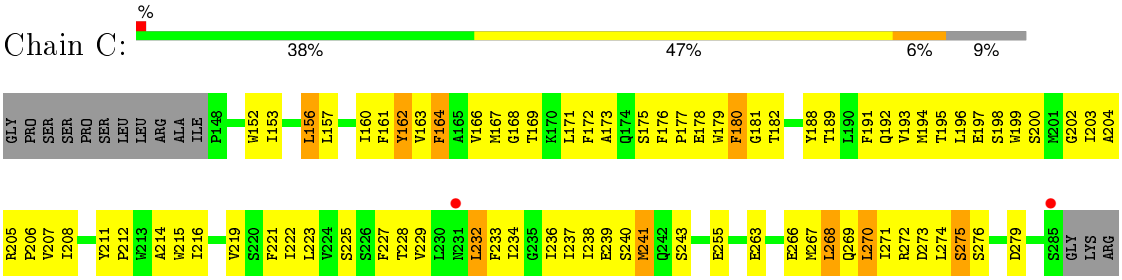
- Molecule 1: Ion transport protein

Chain B:



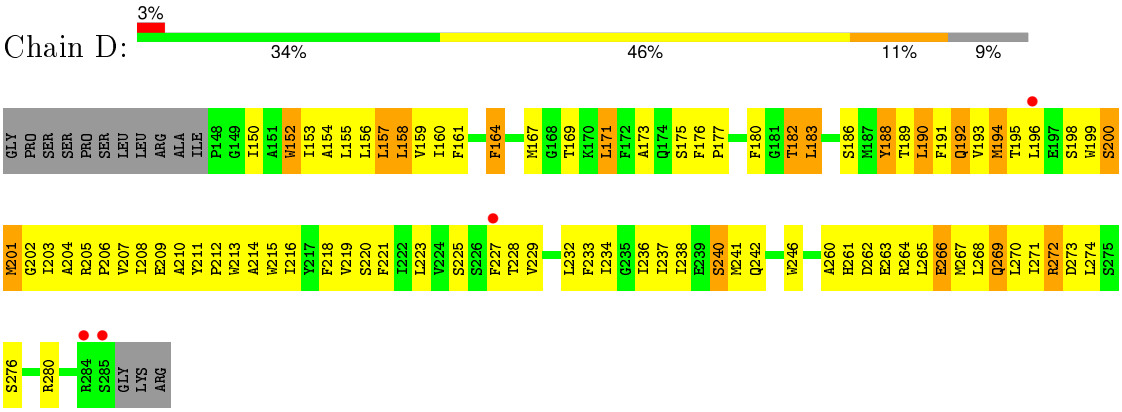
- Molecule 1: Ion transport protein

Chain C:



- Molecule 1: Ion transport protein

Chain D:


3%
34%
46%
11%
9%
GLY PRO SER SER PRO SER LEU LEU ARG ALA ILE P148 G149 I150 A151 W152 I153 A154 L155 L156 L157 L158 V159 I160 F161 F164 M167 G168 T169 K170 L171 F172 A173 Q174 S175 F176 P177 F180 G181 T182 L183 S186 M187 Y188 T189 L190 F191 Q192 V193 M194 T195 L196 E197 S198 W199 S200
M201 G202 I203 A204 R205 P206 V207 I208 E209 A210 Y211 P212 W213 A214 W215 I216 Y217 F218 V219 S220 F221 I222 L223 V224 S225 S226 F227 T228 V229 L232 F233 I234 G235 I236 I237 I238 E239 S240 M241 Q242 W246 A260 H261 D262 E263 R264 L265 E266 M267 L268 Q269 L270 I271 R272 D273 L274 S275
S276 R280 R284 S285 GLY LYS ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	147.67Å 161.68Å 162.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.46 73.83 – 3.46	Depositor EDS
% Data completeness (in resolution range)	89.1 (15.00-3.46) 89.2 (73.83-3.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.224 , 0.268 0.223 , 0.266	Depositor DCC
R_{free} test set	1173 reflections (5.47%)	DCC
Wilson B-factor (Å^2)	159.7	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 222.2	EDS
Estimated twinning fraction	0.117 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 22952 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	4095	wwPDB-VP
Average B, all atoms (Å^2)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: NI, CA

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	0.72	3/1057 (0.3%)	0.85	3/1447 (0.2%)
1	B	0.49	0/1053	0.76	2/1442 (0.1%)
1	C	0.54	0/1049	0.76	0/1437
1	D	0.55	0/1038	0.83	1/1423 (0.1%)
All	All	0.58	3/4197 (0.1%)	0.80	6/5749 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	PHE	CG-CD1	5.99	1.47	1.38
1	A	176	PHE	CG-CD2	5.45	1.47	1.38
1	A	176	PHE	CE2-CZ	5.06	1.47	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	196	LEU	CA-CB-CG	5.54	128.05	115.30
1	D	273	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	171	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	A	205	ARG	C-N-CD	5.28	139.48	128.40
1	A	206	PRO	CA-N-CD	-5.22	104.20	111.50
1	B	157	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1029	0	957	152	0
1	B	1025	0	958	101	0
1	C	1020	0	948	121	0
1	D	1010	0	937	151	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
All	All	4095	0	3800	446	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 (446) 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:D:215:TRP:NE1	1:D:216:ILE:HG13	1.47	1.26
1:A:176:PHE:CZ	1:A:210:ALA:HB2	1.82	1.15
1:A:241:MET:HB3	1:D:241:MET:CE	1.77	1.13
1:A:176:PHE:HZ	1:A:210:ALA:HB2	1.03	1.12
1:A:241:MET:HB3	1:D:241:MET:HE1	1.26	1.09
1:B:237:ILE:HA	1:C:234:ILE:HD11	1.09	1.09
1:A:200:SER:OG	1:A:205:ARG:HG2	1.52	1.09
1:D:153:ILE:HG13	1:D:232:LEU:HD12	1.32	1.07
1:A:237:ILE:HA	1:B:234:ILE:HD11	1.26	1.06
1:D:215:TRP:CE2	1:D:216:ILE:HG13	1.89	1.06
1:B:268:LEU:HA	1:B:271:ILE:HD12	1.34	1.04
1:C:176:PHE:CE2	1:C:207:VAL:HA	1.94	1.02
1:A:179:TRP:CZ3	1:A:207:VAL:HG23	1.98	0.99
1:A:238:ILE:HD11	1:D:240:SER:HB3	1.42	0.97
1:A:223:LEU:O	1:A:227:PHE:HB2	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HA	1:B:160:ILE:HD12	1.45	0.95
1:B:237:ILE:CA	1:C:234:ILE:HD11	1.96	0.94
1:D:150:ILE:O	1:D:153:ILE:HG12	1.68	0.94
1:A:167:MET:O	1:A:171:LEU:HB2	1.70	0.92
1:A:157:LEU:HA	1:A:160:ILE:HD12	1.53	0.90
1:D:215:TRP:NE1	1:D:216:ILE:CG1	2.32	0.90
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.53	0.88
1:B:215:TRP:NE1	1:B:216:ILE:HG13	1.88	0.88
1:B:237:ILE:HA	1:C:234:ILE:CD1	2.01	0.88
1:A:241:MET:CB	1:D:241:MET:CE	2.50	0.88
1:B:223:LEU:O	1:B:227:PHE:HB2	1.74	0.87
1:D:190:LEU:HD13	1:D:221:PHE:HE2	1.40	0.87
1:A:176:PHE:CZ	1:A:210:ALA:CB	2.57	0.87
1:D:223:LEU:O	1:D:227:PHE:HB2	1.74	0.86
1:B:169:THR:O	1:B:173:ALA:HB2	1.76	0.86
1:A:215:TRP:NE1	1:A:216:ILE:HG13	1.91	0.85
1:A:179:TRP:HZ3	1:A:207:VAL:HG23	1.41	0.85
1:A:207:VAL:O	1:A:210:ALA:HB3	1.75	0.85
1:A:154:ALA:O	1:A:158:LEU:HG	1.76	0.85
1:B:267:MET:SD	1:C:267:MET:CE	2.64	0.85
1:B:215:TRP:CE2	1:B:216:ILE:HG13	2.12	0.85
1:A:237:ILE:O	1:A:241:MET:HB2	1.77	0.83
1:A:241:MET:CB	1:D:241:MET:HE3	2.10	0.82
1:A:203:ILE:O	1:A:207:VAL:HG23	1.80	0.82
1:A:215:TRP:O	1:A:219:VAL:HG23	1.80	0.81
1:B:262:ASP:O	1:B:266:GLU:HB3	1.81	0.80
1:C:192:GLN:NE2	1:D:205:ARG:HH21	1.78	0.80
1:C:197:GLU:HG3	1:D:199:TRP:H	1.47	0.80
1:C:179:TRP:HZ3	1:C:207:VAL:HG23	1.45	0.80
1:C:223:LEU:O	1:C:227:PHE:HB2	1.81	0.79
1:C:208:ILE:HA	1:C:211:TYR:O	1.81	0.79
1:A:208:ILE:HG12	1:A:214:ALA:HB3	1.64	0.79
1:D:176:PHE:CZ	1:D:207:VAL:HA	2.16	0.79
1:B:189:THR:O	1:B:193:VAL:HG23	1.83	0.78
1:C:237:ILE:HA	1:D:234:ILE:HD11	1.65	0.78
1:A:234:ILE:HD11	1:D:237:ILE:HA	1.65	0.78
1:A:237:ILE:HA	1:B:234:ILE:CD1	2.12	0.78
1:A:199:TRP:O	1:A:203:ILE:HB	1.83	0.78
1:C:176:PHE:CD2	1:C:207:VAL:HG22	2.19	0.77
1:D:208:ILE:O	1:D:212:PRO:HA	1.83	0.77
1:D:215:TRP:O	1:D:219:VAL:HG23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ILE:CG1	1:D:232:LEU:HD12	2.12	0.77
1:C:169:THR:O	1:C:173:ALA:HB2	1.84	0.77
1:B:203:ILE:O	1:B:207:VAL:HG23	1.84	0.77
1:A:241:MET:HB3	1:D:241:MET:HE3	1.64	0.76
1:D:153:ILE:HD12	1:D:232:LEU:HA	1.66	0.76
1:A:200:SER:O	1:A:205:ARG:HB2	1.86	0.76
1:D:242:GLN:HA	1:D:246:TRP:CB	2.15	0.76
1:A:153:ILE:HB	1:A:232:LEU:HD12	1.69	0.75
1:D:190:LEU:HD13	1:D:221:PHE:CE2	2.22	0.74
1:A:200:SER:HA	1:A:204:ALA:H	1.50	0.74
1:C:219:VAL:O	1:C:223:LEU:HG	1.86	0.74
1:B:214:ALA:O	1:B:217:TYR:HB3	1.86	0.74
1:C:215:TRP:NE1	1:C:216:ILE:HG13	2.02	0.74
1:C:234:ILE:HG13	1:C:237:ILE:HD12	1.69	0.74
1:D:153:ILE:HD12	1:D:232:LEU:CB	2.17	0.74
1:D:191:PHE:HA	1:D:194:MET:HB2	1.69	0.74
1:D:157:LEU:HD23	1:D:158:LEU:N	2.03	0.73
1:C:193:VAL:HG13	1:C:199:TRP:HB2	1.70	0.73
1:A:211:TYR:HB3	1:A:213:TRP:NE1	2.03	0.73
1:C:197:GLU:CG	1:D:199:TRP:H	2.00	0.73
1:A:225:SER:O	1:A:229:VAL:HG23	1.89	0.72
1:B:267:MET:HG2	1:B:271:ILE:HD11	1.71	0.72
1:D:266:GLU:HA	1:D:269:GLN:HB2	1.72	0.72
1:B:205:ARG:HB2	1:B:206:PRO:HD3	1.71	0.72
1:D:215:TRP:CG	1:D:216:ILE:N	2.58	0.72
1:A:233:PHE:HA	1:A:236:ILE:HD12	1.71	0.72
1:C:266:GLU:O	1:C:269:GLN:HB3	1.89	0.72
1:A:169:THR:O	1:A:173:ALA:HB2	1.90	0.72
1:B:208:ILE:HD11	1:B:215:TRP:HA	1.70	0.71
1:B:215:TRP:O	1:B:219:VAL:HG23	1.90	0.71
1:A:236:ILE:O	1:A:240:SER:HB2	1.91	0.70
1:A:204:ALA:HA	1:A:207:VAL:HB	1.73	0.70
1:D:267:MET:O	1:D:271:ILE:HG13	1.92	0.70
1:C:197:GLU:OE1	1:D:198:SER:HA	1.92	0.70
1:C:192:GLN:HG3	1:D:200:SER:HB3	1.74	0.70
1:D:153:ILE:HD12	1:D:232:LEU:CA	2.22	0.69
1:D:215:TRP:CD1	1:D:216:ILE:HG13	2.24	0.69
1:C:171:LEU:HB2	1:C:172:PHE:CD1	2.27	0.69
1:B:267:MET:SD	1:C:267:MET:HE2	2.33	0.69
1:B:263:GLU:HA	1:B:266:GLU:HG2	1.74	0.69
1:A:237:ILE:CA	1:B:234:ILE:HD11	2.15	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LEU:HA	1:C:271:ILE:HD12	1.74	0.69
1:C:171:LEU:HD12	1:C:172:PHE:CE1	2.28	0.68
1:B:176:PHE:CZ	1:B:207:VAL:HA	2.29	0.68
1:B:233:PHE:CE2	1:B:237:ILE:HD11	2.29	0.68
1:D:219:VAL:O	1:D:223:LEU:HG	1.94	0.68
1:C:241:MET:HE3	1:D:241:MET:HB2	1.76	0.68
1:A:232:LEU:HD23	1:A:236:ILE:HD11	1.75	0.67
1:D:215:TRP:HE1	1:D:216:ILE:CD1	2.08	0.67
1:D:233:PHE:HA	1:D:236:ILE:HD12	1.75	0.67
1:D:176:PHE:CE2	1:D:207:VAL:HA	2.29	0.67
1:A:177:PRO:HA	1:A:181:GLY:CA	2.26	0.66
1:A:176:PHE:CE2	1:A:210:ALA:CB	2.79	0.66
1:C:172:PHE:CD2	1:C:207:VAL:HG13	2.30	0.66
1:C:176:PHE:HE2	1:C:207:VAL:HA	1.55	0.66
1:A:241:MET:HB2	1:D:241:MET:HE3	1.78	0.66
1:A:179:TRP:CZ3	1:A:207:VAL:CG2	2.77	0.66
1:A:219:VAL:O	1:A:223:LEU:HG	1.96	0.66
1:B:215:TRP:CG	1:B:216:ILE:N	2.64	0.66
1:A:204:ALA:O	1:A:208:ILE:HB	1.96	0.65
1:B:240:SER:HB3	1:C:238:ILE:HD11	1.78	0.65
1:A:162:TYR:O	1:A:166:VAL:HG23	1.96	0.65
1:A:215:TRP:CE2	1:A:216:ILE:HG13	2.32	0.65
1:A:200:SER:O	1:A:205:ARG:CB	2.45	0.65
1:A:211:TYR:HB3	1:A:213:TRP:CD1	2.31	0.65
1:A:156:LEU:O	1:A:160:ILE:HG13	1.95	0.65
1:D:269:GLN:HA	1:D:269:GLN:HE21	1.60	0.65
1:D:268:LEU:HB3	1:D:272:ARG:HH22	1.62	0.64
1:B:196:LEU:HA	1:B:199:TRP:HB3	1.79	0.64
1:A:172:PHE:HB2	1:A:180:PHE:CD2	2.33	0.64
1:A:204:ALA:HB1	1:A:218:PHE:CD1	2.33	0.64
1:C:195:THR:HB	1:D:196:LEU:HD13	1.79	0.64
1:C:164:PHE:CD2	1:C:221:PHE:HD1	2.15	0.64
1:C:164:PHE:CE2	1:C:221:PHE:HA	2.32	0.63
1:D:204:ALA:O	1:D:208:ILE:HB	1.97	0.63
1:C:263:GLU:OE2	1:D:261:HIS:CD2	2.51	0.63
1:C:237:ILE:O	1:C:241:MET:HB2	1.99	0.63
1:A:203:ILE:HG22	1:A:218:PHE:CE2	2.34	0.63
1:A:203:ILE:CG2	1:A:218:PHE:CE2	2.82	0.62
1:D:153:ILE:CD1	1:D:232:LEU:HA	2.28	0.62
1:B:208:ILE:HA	1:B:211:TYR:O	1.99	0.62
1:B:194:MET:O	1:B:196:LEU:HD23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:SER:O	1:B:229:VAL:HG23	2.00	0.62
1:C:177:PRO:HD2	1:C:178:GLU:H	1.63	0.62
1:A:241:MET:CB	1:D:241:MET:HE1	2.14	0.62
1:A:208:ILE:CG1	1:A:214:ALA:HB3	2.29	0.62
1:C:172:PHE:CE2	1:C:207:VAL:CG1	2.82	0.62
1:D:264:ARG:O	1:D:268:LEU:HB2	2.00	0.62
1:C:171:LEU:HD12	1:C:172:PHE:HE1	1.63	0.62
1:A:183:LEU:HD13	1:A:187:MET:HG2	1.82	0.61
1:C:233:PHE:CE2	1:C:237:ILE:HD11	2.35	0.61
1:D:164:PHE:CE2	1:D:221:PHE:HA	2.35	0.61
1:D:205:ARG:HB2	1:D:206:PRO:HD3	1.82	0.61
1:D:215:TRP:CD1	1:D:216:ILE:N	2.66	0.61
1:A:196:LEU:HD13	1:D:195:THR:HB	1.83	0.61
1:D:182:THR:OG1	1:D:183:LEU:N	2.34	0.61
1:A:207:VAL:HG11	1:A:218:PHE:CZ	2.36	0.60
1:D:204:ALA:HA	1:D:218:PHE:CE2	2.36	0.60
1:D:157:LEU:HA	1:D:160:ILE:HD12	1.83	0.60
1:D:167:MET:O	1:D:171:LEU:HD13	2.01	0.60
1:D:152:TRP:HA	1:D:152:TRP:CE3	2.36	0.60
1:A:214:ALA:O	1:A:217:TYR:HB3	2.02	0.60
1:B:201:MET:HA	1:B:205:ARG:HG3	1.83	0.60
1:C:179:TRP:CZ3	1:C:207:VAL:HG23	2.33	0.60
1:C:168:GLY:O	1:C:172:PHE:HD1	1.84	0.60
1:D:236:ILE:O	1:D:240:SER:HB2	2.01	0.60
1:A:179:TRP:CE3	1:A:207:VAL:HG23	2.37	0.60
1:A:204:ALA:O	1:A:208:ILE:HD12	2.02	0.60
1:A:176:PHE:HZ	1:A:210:ALA:CB	1.91	0.59
1:B:172:PHE:HB3	1:B:176:PHE:HD2	1.67	0.59
1:C:241:MET:CE	1:D:241:MET:HB2	2.32	0.59
1:A:156:LEU:O	1:A:159:VAL:HB	2.03	0.59
1:C:275:SER:O	1:C:279:ASP:CB	2.51	0.59
1:A:204:ALA:HB2	1:A:218:PHE:CD2	2.37	0.59
1:A:274:LEU:HD21	1:B:275:SER:OG	2.03	0.59
1:B:197:GLU:OE1	1:C:198:SER:HA	2.01	0.59
1:C:202:GLY:O	1:C:206:PRO:HG2	2.03	0.59
1:B:199:TRP:CZ3	1:B:200:SER:HB2	2.38	0.59
1:A:179:TRP:CE3	1:A:207:VAL:CG2	2.86	0.58
1:A:199:TRP:CZ3	1:A:200:SER:HB2	2.38	0.58
1:D:260:ALA:HA	1:D:263:GLU:HB2	1.84	0.58
1:A:255:GLU:O	1:A:258:GLN:HB3	2.03	0.58
1:C:196:LEU:HA	1:C:199:TRP:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:O	1:B:160:ILE:HG13	2.04	0.58
1:A:267:MET:HE3	1:D:267:MET:SD	2.42	0.58
1:A:237:ILE:O	1:A:241:MET:N	2.36	0.58
1:D:268:LEU:HA	1:D:271:ILE:HD12	1.84	0.58
1:A:203:ILE:O	1:A:207:VAL:CG2	2.52	0.57
1:A:234:ILE:HD11	1:D:237:ILE:CA	2.34	0.57
1:B:267:MET:CG	1:B:271:ILE:HD11	2.33	0.57
1:B:171:LEU:HD23	1:B:213:TRP:CZ3	2.39	0.57
1:B:266:GLU:HG3	1:B:267:MET:N	2.20	0.57
1:D:265:LEU:O	1:D:268:LEU:HB2	2.04	0.57
1:B:229:VAL:O	1:B:233:PHE:N	2.32	0.57
1:B:270:LEU:HG	1:C:271:ILE:HG22	1.85	0.57
1:B:215:TRP:CD1	1:B:216:ILE:N	2.71	0.57
1:A:160:ILE:C	1:A:163:VAL:HG22	2.25	0.57
1:A:219:VAL:HG12	1:A:223:LEU:HD11	1.87	0.57
1:A:160:ILE:HA	1:A:163:VAL:CG2	2.34	0.57
1:A:192:GLN:HG3	1:B:200:SER:CB	2.35	0.57
1:A:267:MET:HG2	1:B:271:ILE:HD13	1.86	0.56
1:D:215:TRP:HE1	1:D:216:ILE:HG13	1.62	0.56
1:C:270:LEU:H	1:C:270:LEU:HD13	1.70	0.56
1:B:215:TRP:NE1	1:B:216:ILE:CG1	2.67	0.56
1:B:260:ALA:HA	1:B:263:GLU:HB3	1.86	0.56
1:B:149:GLY:O	1:B:152:TRP:HB2	2.06	0.56
1:B:233:PHE:HZ	1:C:233:PHE:HE2	1.54	0.56
1:A:268:LEU:HA	1:A:271:ILE:HD12	1.87	0.56
1:C:268:LEU:HD22	1:C:272:ARG:HH12	1.71	0.56
1:C:267:MET:HG3	1:D:268:LEU:HG	1.88	0.56
1:D:189:THR:O	1:D:193:VAL:N	2.35	0.56
1:C:241:MET:HE2	1:D:238:ILE:HG23	1.87	0.55
1:A:203:ILE:C	1:A:206:PRO:HD2	2.26	0.55
1:B:196:LEU:HB3	1:B:199:TRP:HD1	1.70	0.55
1:B:176:PHE:HB3	1:B:179:TRP:CE3	2.41	0.55
1:D:268:LEU:HD22	1:D:272:ARG:HH22	1.72	0.55
1:C:225:SER:O	1:C:229:VAL:HG23	2.06	0.55
1:C:157:LEU:HA	1:C:160:ILE:HD12	1.87	0.55
1:A:229:VAL:O	1:A:233:PHE:N	2.30	0.55
1:C:177:PRO:HA	1:C:181:GLY:HA2	1.88	0.55
1:C:269:GLN:C	1:C:271:ILE:H	2.09	0.55
1:D:204:ALA:O	1:D:208:ILE:N	2.39	0.55
1:A:221:PHE:O	1:A:225:SER:CB	2.55	0.55
1:A:267:MET:CE	1:D:267:MET:SD	2.94	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ILE:O	1:A:240:SER:CB	2.55	0.54
1:D:164:PHE:HE2	1:D:221:PHE:HA	1.71	0.54
1:C:267:MET:HG3	1:D:268:LEU:CD2	2.37	0.54
1:D:188:TYR:HE1	1:D:192:GLN:HG3	1.72	0.54
1:C:197:GLU:HG3	1:D:199:TRP:N	2.20	0.54
1:A:261:HIS:CE1	1:D:263:GLU:OE2	2.61	0.54
1:D:208:ILE:HA	1:D:214:ALA:HB3	1.89	0.54
1:D:225:SER:O	1:D:229:VAL:HG23	2.07	0.54
1:C:177:PRO:CD	1:C:178:GLU:H	2.21	0.54
1:D:213:TRP:O	1:D:216:ILE:HB	2.08	0.54
1:A:179:TRP:HH2	1:A:206:PRO:HB2	1.71	0.54
1:C:172:PHE:CD2	1:C:207:VAL:CG1	2.91	0.54
1:B:199:TRP:CH2	1:B:200:SER:HB2	2.43	0.54
1:C:266:GLU:O	1:C:270:LEU:HD13	2.08	0.54
1:A:238:ILE:HG22	1:A:239:GLU:N	2.23	0.54
1:C:171:LEU:HB2	1:C:172:PHE:CE1	2.43	0.54
1:A:215:TRP:CG	1:A:216:ILE:N	2.75	0.54
1:A:160:ILE:CA	1:A:163:VAL:HG22	2.39	0.53
1:A:267:MET:CG	1:B:271:ILE:HD13	2.38	0.53
1:B:157:LEU:CA	1:B:160:ILE:HD12	2.30	0.53
1:C:193:VAL:O	1:C:196:LEU:HD23	2.09	0.53
1:A:207:VAL:HG11	1:A:218:PHE:CE1	2.44	0.53
1:B:229:VAL:O	1:B:232:LEU:N	2.40	0.53
1:A:204:ALA:HB2	1:A:218:PHE:CG	2.43	0.53
1:D:153:ILE:HD12	1:D:232:LEU:HB2	1.90	0.53
1:D:169:THR:O	1:D:173:ALA:HB2	2.08	0.53
1:A:199:TRP:CZ3	1:A:200:SER:CB	2.92	0.53
1:D:208:ILE:O	1:D:212:PRO:CA	2.56	0.53
1:C:267:MET:HG3	1:D:268:LEU:HD23	1.91	0.53
1:D:268:LEU:HB3	1:D:272:ARG:NH2	2.24	0.52
1:A:215:TRP:CD1	1:A:216:ILE:N	2.77	0.52
1:C:169:THR:O	1:C:173:ALA:CB	2.55	0.52
1:A:232:LEU:CD2	1:A:236:ILE:HD11	2.39	0.52
1:C:203:ILE:O	1:C:207:VAL:HG23	2.10	0.52
1:A:240:SER:HA	1:A:243:SER:OG	2.09	0.52
1:B:241:MET:CE	1:C:241:MET:HB3	2.40	0.52
1:D:188:TYR:C	1:D:188:TYR:CD1	2.82	0.52
1:A:177:PRO:HA	1:A:181:GLY:N	2.25	0.52
1:B:196:LEU:HB3	1:B:199:TRP:CD1	2.44	0.52
1:C:177:PRO:HA	1:C:181:GLY:CA	2.40	0.52
1:B:163:VAL:HG12	1:B:164:PHE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:SER:O	1:A:205:ARG:CG	2.58	0.52
1:D:188:TYR:O	1:D:192:GLN:N	2.41	0.52
1:A:271:ILE:HG21	1:D:270:LEU:HB3	1.91	0.52
1:A:172:PHE:HB3	1:A:176:PHE:HD2	1.75	0.52
1:A:160:ILE:HA	1:A:163:VAL:HG22	1.91	0.52
1:B:191:PHE:HZ	1:C:222:ILE:HG21	1.75	0.52
1:A:234:ILE:HG13	1:A:237:ILE:HD12	1.91	0.52
1:C:241:MET:HE3	1:D:238:ILE:HA	1.91	0.52
1:D:221:PHE:C	1:D:221:PHE:CD1	2.82	0.52
1:D:233:PHE:CE2	1:D:237:ILE:HD11	2.45	0.51
1:B:162:TYR:O	1:B:166:VAL:HG23	2.10	0.51
1:C:180:PHE:N	1:C:180:PHE:CD1	2.78	0.51
1:D:215:TRP:CE2	1:D:216:ILE:CG1	2.79	0.51
1:A:204:ALA:CB	1:A:218:PHE:CD1	2.93	0.51
1:D:208:ILE:HG22	1:D:209:GLU:N	2.24	0.51
1:D:154:ALA:O	1:D:158:LEU:HB2	2.10	0.51
1:B:157:LEU:HD11	1:B:229:VAL:HG22	1.93	0.51
1:B:155:LEU:O	1:B:159:VAL:N	2.41	0.50
1:A:220:SER:HA	1:A:223:LEU:HD12	1.92	0.50
1:A:157:LEU:O	1:A:160:ILE:HB	2.11	0.50
1:C:208:ILE:HD11	1:C:215:TRP:HA	1.93	0.50
1:B:204:ALA:HA	1:B:218:PHE:CE2	2.47	0.49
1:B:267:MET:SD	1:C:267:MET:HE3	2.52	0.49
1:D:220:SER:HA	1:D:223:LEU:HD12	1.93	0.49
1:B:150:ILE:C	1:B:152:TRP:H	2.15	0.49
1:D:150:ILE:C	1:D:152:TRP:N	2.65	0.49
1:A:152:TRP:CE3	1:A:152:TRP:HA	2.47	0.49
1:C:215:TRP:CG	1:C:216:ILE:N	2.80	0.49
1:A:153:ILE:HD13	1:A:232:LEU:HA	1.94	0.49
1:B:197:GLU:OE2	1:C:200:SER:HB3	2.12	0.49
1:A:192:GLN:HG3	1:B:200:SER:HB3	1.93	0.49
1:A:221:PHE:O	1:A:225:SER:HB3	2.13	0.48
1:A:271:ILE:CG2	1:D:270:LEU:HB3	2.43	0.48
1:C:205:ARG:HB2	1:C:206:PRO:HD3	1.95	0.48
1:C:267:MET:HB2	1:D:268:LEU:HD21	1.95	0.48
1:C:179:TRP:HZ3	1:C:207:VAL:CG2	2.20	0.48
1:C:197:GLU:OE1	1:D:201:MET:HB2	2.13	0.48
1:C:197:GLU:HG3	1:D:199:TRP:CD1	2.48	0.48
1:C:269:GLN:HE22	1:C:273:ASP:CB	2.26	0.48
1:C:274:LEU:C	1:C:276:SER:H	2.16	0.48
1:C:268:LEU:O	1:C:271:ILE:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ILE:HD11	1:B:215:TRP:CA	2.42	0.48
1:B:272:ARG:O	1:B:275:SER:HB2	2.14	0.47
1:C:268:LEU:CA	1:C:271:ILE:HD12	2.44	0.47
1:B:154:ALA:O	1:B:158:LEU:N	2.46	0.47
1:D:229:VAL:O	1:D:233:PHE:N	2.34	0.47
1:D:220:SER:O	1:D:221:PHE:C	2.51	0.47
1:A:186:SER:O	1:A:190:LEU:N	2.28	0.47
1:A:270:LEU:HD21	1:B:272:ARG:HG3	1.97	0.47
1:D:169:THR:O	1:D:173:ALA:CB	2.62	0.47
1:C:215:TRP:CE2	1:C:216:ILE:HG13	2.49	0.47
1:D:152:TRP:HA	1:D:152:TRP:HE3	1.79	0.47
1:A:171:LEU:HD21	1:A:213:TRP:CZ2	2.50	0.47
1:C:233:PHE:HA	1:C:236:ILE:CD1	2.36	0.47
1:C:237:ILE:O	1:C:241:MET:CB	2.62	0.47
1:A:211:TYR:HB2	1:A:214:ALA:HB2	1.97	0.47
1:C:162:TYR:O	1:C:166:VAL:HG23	2.15	0.47
1:B:156:LEU:O	1:B:159:VAL:HB	2.15	0.47
1:A:215:TRP:NE1	1:A:216:ILE:CG1	2.74	0.47
1:A:241:MET:SD	1:D:241:MET:HE1	2.55	0.46
1:D:191:PHE:HA	1:D:194:MET:CB	2.43	0.46
1:D:211:TYR:O	1:D:214:ALA:CB	2.63	0.46
1:C:160:ILE:HD11	1:C:228:THR:HG21	1.98	0.46
1:C:167:MET:O	1:C:171:LEU:HG	2.15	0.46
1:C:208:ILE:HG13	1:C:214:ALA:HB3	1.98	0.46
1:D:264:ARG:HA	1:D:267:MET:HB3	1.98	0.46
1:B:202:GLY:O	1:B:206:PRO:HG2	2.16	0.46
1:C:267:MET:CG	1:D:268:LEU:HG	2.45	0.46
1:C:189:THR:O	1:C:192:GLN:HB3	2.15	0.46
1:A:203:ILE:CG2	1:A:218:PHE:HE2	2.29	0.45
1:B:153:ILE:O	1:B:157:LEU:HB3	2.17	0.45
1:A:259:ARG:HA	1:A:262:ASP:HB2	1.97	0.45
1:C:234:ILE:CG1	1:C:237:ILE:HD12	2.43	0.45
1:C:267:MET:HG3	1:D:268:LEU:CG	2.47	0.45
1:B:153:ILE:HG13	1:B:153:ILE:H	1.49	0.45
1:B:234:ILE:HG13	1:B:237:ILE:HD12	1.99	0.45
1:D:188:TYR:HD1	1:D:188:TYR:C	2.19	0.45
1:A:159:VAL:O	1:A:163:VAL:HG13	2.17	0.45
1:B:150:ILE:C	1:B:152:TRP:N	2.69	0.45
1:B:205:ARG:O	1:B:209:GLU:N	2.35	0.45
1:C:192:GLN:HE21	1:D:205:ARG:HH21	1.61	0.45
1:C:239:GLU:O	1:C:243:SER:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:SER:HA	1:D:204:ALA:HB3	1.98	0.45
1:B:164:PHE:HD1	1:B:217:TYR:CE1	2.35	0.45
1:B:236:ILE:O	1:B:240:SER:HB2	2.17	0.45
1:A:193:VAL:O	1:A:196:LEU:HD23	2.17	0.45
1:A:179:TRP:HZ3	1:A:207:VAL:CG2	2.18	0.45
1:A:202:GLY:O	1:A:206:PRO:HG2	2.16	0.45
1:C:215:TRP:CD1	1:C:216:ILE:N	2.84	0.45
1:D:221:PHE:CE1	1:D:225:SER:HB2	2.52	0.44
1:D:268:LEU:HD22	1:D:272:ARG:NH2	2.32	0.44
1:A:172:PHE:CB	1:A:180:PHE:CD2	2.99	0.44
1:A:172:PHE:HB2	1:A:180:PHE:HB2	1.98	0.44
1:D:203:ILE:O	1:D:207:VAL:HG23	2.16	0.44
1:A:234:ILE:HD11	1:D:237:ILE:N	2.32	0.44
1:C:197:GLU:CG	1:D:199:TRP:N	2.75	0.44
1:A:197:GLU:OE2	1:B:200:SER:HB3	2.18	0.44
1:B:191:PHE:CE2	1:C:199:TRP:CZ2	3.06	0.44
1:D:150:ILE:O	1:D:153:ILE:N	2.46	0.44
1:C:175:SER:C	1:C:177:PRO:HD3	2.38	0.44
1:A:237:ILE:O	1:A:241:MET:CB	2.58	0.44
1:D:234:ILE:HG13	1:D:237:ILE:HD12	1.99	0.44
1:D:161:PHE:CZ	1:D:191:PHE:HB2	2.52	0.44
1:D:276:SER:O	1:D:280:ARG:N	2.43	0.44
1:D:269:GLN:HA	1:D:269:GLN:NE2	2.30	0.43
1:C:153:ILE:HG23	1:C:156:LEU:CD2	2.48	0.43
1:D:164:PHE:HD1	1:D:164:PHE:HA	1.68	0.43
1:A:207:VAL:HG11	1:A:218:PHE:HZ	1.81	0.43
1:C:188:TYR:O	1:C:189:THR:C	2.57	0.43
1:D:196:LEU:HA	1:D:199:TRP:HB3	2.00	0.43
1:D:171:LEU:N	1:D:171:LEU:CD1	2.81	0.43
1:D:173:ALA:HA	1:D:180:PHE:C	2.39	0.43
1:B:215:TRP:HE1	1:B:216:ILE:CD1	2.32	0.43
1:B:221:PHE:O	1:B:225:SER:HB3	2.18	0.43
1:B:229:VAL:O	1:B:230:LEU:C	2.57	0.43
1:A:200:SER:O	1:A:205:ARG:HG2	2.18	0.43
1:A:271:ILE:O	1:A:274:LEU:HB2	2.18	0.43
1:C:172:PHE:N	1:C:172:PHE:CD1	2.86	0.43
1:A:204:ALA:O	1:A:208:ILE:CB	2.65	0.43
1:B:267:MET:HA	1:C:268:LEU:HD21	2.01	0.43
1:A:176:PHE:CZ	1:A:207:VAL:HA	2.54	0.43
1:B:197:GLU:HG3	1:C:199:TRP:CD1	2.54	0.43
1:B:203:ILE:O	1:B:207:VAL:CG2	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:LEU:HD21	1:D:274:LEU:HG	2.01	0.42
1:B:151:ALA:O	1:B:154:ALA:HB3	2.19	0.42
1:C:153:ILE:HG21	1:C:232:LEU:HB2	2.01	0.42
1:D:156:LEU:O	1:D:159:VAL:HB	2.19	0.42
1:A:274:LEU:CD2	1:B:275:SER:OG	2.65	0.42
1:B:176:PHE:CE2	1:B:207:VAL:HA	2.54	0.42
1:D:260:ALA:C	1:D:262:ASP:N	2.70	0.42
1:A:237:ILE:HG22	1:A:241:MET:HG3	2.00	0.42
1:A:180:PHE:HD1	1:A:186:SER:OG	2.02	0.42
1:A:161:PHE:HZ	1:A:191:PHE:HA	1.84	0.42
1:D:215:TRP:CE3	1:D:219:VAL:HG21	2.55	0.42
1:C:267:MET:SD	1:D:268:LEU:HG	2.60	0.42
1:D:204:ALA:CB	1:D:218:PHE:CD2	3.03	0.42
1:A:171:LEU:CD2	1:A:213:TRP:CZ2	3.02	0.42
1:A:149:GLY:H	1:A:152:TRP:HB2	1.85	0.42
1:D:211:TYR:O	1:D:214:ALA:HB2	2.20	0.42
1:B:191:PHE:HE2	1:C:199:TRP:CZ2	2.38	0.42
1:A:275:SER:OG	1:D:274:LEU:HD13	2.20	0.42
1:B:234:ILE:HA	1:B:237:ILE:HD12	2.00	0.42
1:A:205:ARG:HE	1:D:192:GLN:HE21	1.66	0.42
1:D:198:SER:OG	4:D:401:HOH:O	2.21	0.42
1:A:231:ASN:O	1:A:234:ILE:HG22	2.20	0.42
1:C:237:ILE:CA	1:D:234:ILE:HD11	2.42	0.42
1:B:195:THR:HB	1:C:196:LEU:HD13	2.02	0.41
1:D:153:ILE:HD11	1:D:232:LEU:HG	2.02	0.41
1:C:263:GLU:OE2	1:D:261:HIS:CG	2.72	0.41
1:A:222:ILE:O	1:A:226:SER:N	2.51	0.41
1:A:237:ILE:HG13	1:A:237:ILE:H	1.68	0.41
1:D:265:LEU:O	1:D:269:GLN:HG2	2.19	0.41
1:D:173:ALA:HA	1:D:180:PHE:O	2.21	0.41
1:A:204:ALA:CB	1:A:218:PHE:CG	3.03	0.41
1:A:267:MET:O	1:A:270:LEU:HB2	2.21	0.41
1:D:175:SER:HG	1:D:211:TYR:HE2	1.68	0.41
1:A:168:GLY:HA2	1:A:172:PHE:HD2	1.86	0.41
1:D:202:GLY:C	1:D:203:ILE:HD13	2.41	0.41
1:D:183:LEU:O	1:D:186:SER:HB2	2.20	0.41
1:B:238:ILE:O	1:B:242:GLN:N	2.34	0.41
1:B:280:ARG:O	1:B:284:ARG:CB	2.69	0.41
1:C:191:PHE:CE2	1:D:219:VAL:HG13	2.55	0.41
1:D:153:ILE:HD12	1:D:232:LEU:CG	2.50	0.41
1:C:269:GLN:C	1:C:271:ILE:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:HG12	1:C:164:PHE:N	2.36	0.41
1:B:161:PHE:HD1	1:B:161:PHE:HA	1.81	0.41
1:C:234:ILE:HA	1:C:237:ILE:HD12	2.02	0.41
1:A:168:GLY:HA2	1:A:172:PHE:CD2	2.56	0.41
1:A:179:TRP:CZ3	1:A:203:ILE:O	2.74	0.41
1:A:176:PHE:CE2	1:A:210:ALA:HB3	2.54	0.41
1:C:208:ILE:O	1:C:212:PRO:HA	2.20	0.41
1:A:164:PHE:CE2	1:A:221:PHE:HA	2.56	0.41
1:D:190:LEU:HD23	1:D:190:LEU:HA	1.68	0.41
1:B:161:PHE:O	1:B:162:TYR:C	2.59	0.41
1:A:267:MET:HE2	1:D:267:MET:SD	2.61	0.40
1:C:204:ALA:O	1:C:208:ILE:N	2.38	0.40
1:D:176:PHE:HZ	1:D:210:ALA:HB3	1.86	0.40
1:A:194:MET:HG2	1:A:225:SER:OG	2.21	0.40
1:B:151:ALA:HA	1:B:154:ALA:HB3	2.02	0.40
1:B:241:MET:HE1	1:C:241:MET:HB3	2.03	0.40
1:A:169:THR:HA	1:A:180:PHE:O	2.22	0.40
1:B:219:VAL:O	1:B:223:LEU:HG	2.20	0.40
1:A:161:PHE:CE1	1:A:190:LEU:HB3	2.57	0.40
1:D:153:ILE:CD1	1:D:232:LEU:HG	2.51	0.40
1:C:157:LEU:O	1:C:160:ILE:HB	2.21	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	136/152 (90%)	115 (85%)	21 (15%)	0	100	100
1	B	136/152 (90%)	118 (87%)	18 (13%)	0	100	100
1	C	136/152 (90%)	113 (83%)	23 (17%)	0	100	100
1	D	136/152 (90%)	123 (90%)	13 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	544/608 (90%)	469 (86%)	75 (14%)	0	100 100

There are no Ramachandran outliers to report.

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	96/131 (73%)	72 (75%)	24 (25%)	1 4
1	B	95/131 (72%)	79 (83%)	16 (17%)	2 14
1	C	93/131 (71%)	78 (84%)	15 (16%)	3 17
1	D	91/131 (70%)	71 (78%)	20 (22%)	1 5
All	All	375/524 (72%)	300 (80%)	75 (20%)	1 7

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	TRP
1	A	153	ILE
1	A	155	LEU
1	A	156	LEU
1	A	161	PHE
1	A	164	PHE
1	A	171	LEU
1	A	175	SER
1	A	182	THR
1	A	183	LEU
1	A	190	LEU
1	A	194	MET
1	A	200	SER
1	A	203	ILE
1	A	223	LEU
1	A	229	VAL
1	A	237	ILE

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Mol	Chain	Res	Type
1	A	240	SER
1	A	241	MET
1	A	255	GLU
1	A	262	ASP
1	A	266	GLU
1	A	268	LEU
1	A	279	ASP
1	B	152	TRP
1	B	153	ILE
1	B	155	LEU
1	B	156	LEU
1	B	158	LEU
1	B	161	PHE
1	B	163	VAL
1	B	174	GLN
1	B	194	MET
1	B	196	LEU
1	B	198	SER
1	B	225	SER
1	B	240	SER
1	B	266	GLU
1	B	267	MET
1	B	275	SER
1	C	152	TRP
1	C	156	LEU
1	C	161	PHE
1	C	162	TYR
1	C	164	PHE
1	C	180	PHE
1	C	182	THR
1	C	194	MET
1	C	232	LEU
1	C	240	SER
1	C	241	MET
1	C	255	GLU
1	C	268	LEU
1	C	270	LEU
1	C	275	SER
1	D	152	TRP
1	D	155	LEU
1	D	157	LEU
1	D	158	LEU

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Mol	Chain	Res	Type
1	D	164	PHE
1	D	171	LEU
1	D	177	PRO
1	D	182	THR
1	D	183	LEU
1	D	188	TYR
1	D	190	LEU
1	D	192	GLN
1	D	194	MET
1	D	200	SER
1	D	201	MET
1	D	228	THR
1	D	240	SER
1	D	266	GLU
1	D	269	GLN
1	D	272	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	261	HIS
1	B	231	ASN
1	C	192	GLN
1	C	269	GLN
1	D	192	GLN
1	D	231	ASN
1	D	269	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

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	138/152 (90%)	-0.13	3 (2%)	65	59	54, 193, 260, 400	0
1	B	138/152 (90%)	-0.17	5 (3%)	46	40	130, 195, 276, 313	0
1	C	138/152 (90%)	-0.24	2 (1%)	78	71	112, 185, 246, 349	0
1	D	138/152 (90%)	-0.05	4 (2%)	55	48	114, 178, 249, 317	0
All	All	552/608 (90%)	-0.15	14 (2%)	61	54	54, 188, 265, 400	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	285	SER	6.4
1	A	285	SER	5.6
1	C	285	SER	4.5
1	D	284	ARG	3.8
1	A	284	ARG	3.2
1	A	282	GLU	3.2
1	C	231	ASN	3.2
1	B	285	SER	2.9
1	B	199	TRP	2.8
1	B	201	MET	2.7
1	B	242	GLN	2.5
1	D	227	PHE	2.5
1	D	196	LEU	2.3
1	B	183	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	B	301	1/1	0.97	0.39	-	113,113,113,113	0
2	CA	D	301	1/1	0.82	0.82	-	178,178,178,178	0
2	CA	A	301	1/1	0.83	0.27	-	212,212,212,212	0
2	CA	B	302	1/1	0.99	0.36	-	145,145,145,145	0
2	CA	B	303	1/1	0.46	1.19	-	234,234,234,234	0
3	NI	A	303	1/1	0.99	0.54	-	146,146,146,146	0
2	CA	A	302	1/1	0.99	0.41	-	180,180,180,180	0

6.5 Other polymers (i)

There are no such residues in this entry.