



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:19 AM UTC

PDB ID : 4LTO / pdb_00004lto
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

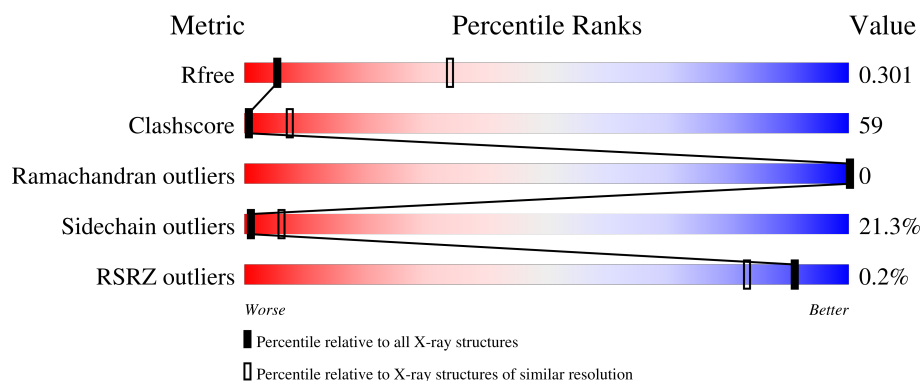
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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

Mol	Chain	Length	Quality of chain
1	A	152	
1	B	152	
1	C	152	
1	D	152	

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 (CCD ID: CA) (formula: Ca).

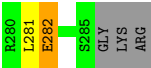
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	3	Total Ca 3 3	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

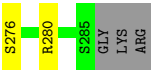
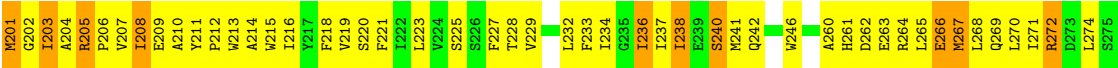
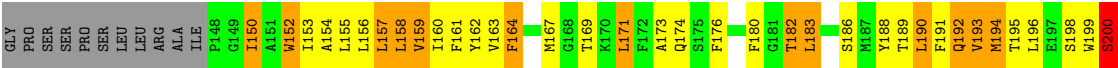
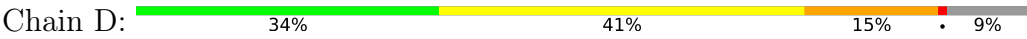
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

- 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



● Molecule 1: Ion transport protein



4 Data and refinement statistics

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 15.00 – 3.46	Depositor EDS
% Data completeness (in resolution range)	89.1 (15.00-3.46) 88.0 (15.00-3.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.224 , 0.268 0.255 , 0.301	Depositor DCC
R_{free} test set	1186 reflections (4.60%)	wwPDB-VP
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 , 242.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.117 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	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.*

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 ⓘ

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

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	0.88	3/1057 (0.3%)	1.32	9/1447 (0.6%)
1	B	0.66	0/1053	1.17	6/1442 (0.4%)
1	C	0.72	0/1049	1.28	10/1437 (0.7%)
1	D	0.71	0/1038	1.27	10/1423 (0.7%)
All	All	0.75	3/4197 (0.1%)	1.26	35/5749 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ARG	C-N	5.79	1.41	1.34
1	A	210	ALA	CA-C	5.50	1.60	1.52
1	A	203	ILE	CA-CB	5.02	1.61	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ALA	N-CA-C	-9.36	101.55	113.72
1	A	282	GLU	N-CA-C	-8.97	101.50	111.28
1	C	261	HIS	N-CA-C	-8.17	102.35	111.82
1	D	203	ILE	N-CA-C	8.07	119.06	111.48
1	A	254	ILE	N-CA-C	-7.18	103.52	110.42
1	C	211	TYR	CA-C-N	6.73	126.18	118.85
1	C	211	TYR	C-N-CA	6.73	126.18	118.85
1	C	176	PHE	CA-C-N	6.55	127.48	120.47
1	C	176	PHE	C-N-CA	6.55	127.48	120.47
1	B	149	GLY	N-CA-C	6.11	118.39	110.45
1	A	209	GLU	N-CA-C	-6.00	104.81	111.71
1	C	203	ILE	CB-CA-C	-5.99	106.62	111.71
1	A	171	LEU	N-CA-C	5.91	120.99	113.55
1	C	247	GLU	N-CA-C	-5.79	104.88	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	150	ILE	CB-CA-C	-5.65	104.72	110.88
1	B	282	GLU	N-CA-C	-5.63	104.55	111.75
1	D	267	MET	N-CA-C	-5.62	104.79	111.03
1	D	193	VAL	CB-CA-C	-5.61	104.47	112.22
1	C	244	ALA	N-CA-C	5.61	119.87	111.96
1	D	193	VAL	N-CA-C	5.59	116.36	110.72
1	B	211	TYR	CA-C-N	5.58	124.94	118.85
1	B	211	TYR	C-N-CA	5.58	124.94	118.85
1	A	206	PRO	CA-N-CD	-5.57	104.20	112.00
1	D	203	ILE	CB-CA-C	-5.55	107.00	111.71
1	D	200	SER	CA-C-N	5.44	127.83	120.65
1	D	200	SER	C-N-CA	5.44	127.83	120.65
1	B	268	LEU	N-CA-C	5.40	117.86	111.33
1	C	282	GLU	N-CA-C	-5.33	106.04	112.54
1	D	205	ARG	CA-C-N	-5.29	113.46	119.28
1	D	205	ARG	C-N-CA	-5.29	113.46	119.28
1	C	281	LEU	N-CA-C	5.16	120.23	113.88
1	A	199	TRP	N-CA-C	5.14	117.55	111.33
1	A	211	TYR	CA-C-N	5.13	124.63	119.19
1	A	211	TYR	C-N-CA	5.13	124.63	119.19
1	B	261	HIS	N-CA-C	-5.08	106.34	112.54

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	1029	0	957	156	0
1	B	1025	0	958	107	0
1	C	1020	0	948	127	0
1	D	1010	0	937	154	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	465	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 59.

All (465) 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: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:A:241:MET:HB3	1:D:241:MET:HE1	1.07	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:241:MET:CB	1:D:241:MET:HE1	1.92	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
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:B:215:TRP:NE1	1:B:216:ILE:HG13	1.88	0.88
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:ALA:O	1:A:158:LEU:HG	1.76	0.85
1:A:207:VAL:O	1:A:210:ALA:HB3	1.75	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:B:215:TRP:CD1	1:B:216:ILE:H	1.97	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:D:215:TRP:CD1	1:D:216:ILE:H	1.98	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
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: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:A:200:SER:HA	1:A:204:ALA:H	1.50	0.74
1:B:214:ALA:O	1:B:217:TYR:HB3	1.86	0.74
1:C:219:VAL:O	1:C:223:LEU:HG	1.86	0.74
1:D:190:LEU:HD13	1:D:221:PHE:CE2	2.22	0.74
1:C:215:TRP:NE1	1:C:216:ILE:HG13	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:193:VAL:HG13	1:C:199:TRP:HB2	1.70	0.73
1:D:157:LEU:HD23	1:D:158:LEU:N	2.03	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:205:ARG:HB2	1:B:206:PRO:HD3	1.71	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: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:241:MET:HE1	1:D:241:MET:HB2	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:B:241:MET:HE1	1:C:241:MET:HB3	1.72	0.70
1:C:241:MET:HE1	1:D:241:MET:CB	2.21	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: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
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:A:267:MET:HE3	1:D:267:MET:SD	2.34	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: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:215:TRP:CD1	1:A:216:ILE:H	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:162:TYR:O	1:A:166:VAL:HG23	1.96	0.65
1:B:240:SER:HB3	1:C:238:ILE:HD11	1.78	0.65
1:A:215:TRP:CE2	1:A:216:ILE:HG13	2.32	0.65
1:A:156:LEU:O	1:A:160:ILE:HG13	1.95	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:D:269:GLN:HE21	1:D:269:GLN:HA	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:C:241:MET:HE3	1:D:238:ILE:HA	1.80	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:B:267:MET:SD	1:C:267:MET:HE2	2.38	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:194:MET:O	1:B:196:LEU:HD23	1.98	0.62
1:B:208:ILE:HA	1:B:211:TYR:O	1.99	0.62
1:C:215:TRP:CD1	1:C:216:ILE:H	2.17	0.62
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: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:C:171:LEU:HD12	1:C:172:PHE:HE1	1.63	0.62
1:D:264:ARG:O	1:D:268:LEU:HB2	2.00	0.62
1:A:183:LEU:HD13	1:A:187:MET:HG2	1.82	0.61
1:A:160:ILE:C	1:A:163:VAL:HG22	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:269:GLN:C	1:C:271:ILE:H	2.09	0.61
1:A:196:LEU:HD13	1:D:195:THR:HB	1.83	0.61
1:D:215:TRP:CD1	1:D:216:ILE:N	2.66	0.61
1:D:182:THR:OG1	1:D:183:LEU:N	2.34	0.61
1:A:194:MET:HE2	1:A:194:MET:O	2.01	0.60
1:A:207:VAL:HG11	1:A:218:PHE:CZ	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:204:ALA:HA	1:D:218:PHE:CE2	2.36	0.60
1:D:152:TRP:HA	1:D:152:TRP:CE3	2.36	0.60
1:A:203:ILE:C	1:A:206:PRO:HD2	2.26	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:A:179:TRP:CE3	1:A:207:VAL:HG23	2.37	0.60
1:D:236:ILE:O	1:D:240:SER:HB2	2.01	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:A:241:MET:CB	1:D:241:MET:HE3	2.33	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:A:255:GLU:O	1:A:258:GLN:HB3	2.03	0.58
1:D:260:ALA:HA	1:D:263:GLU:HB2	1.84	0.58
1:C:196:LEU:HA	1:C:199:TRP:HB3	1.86	0.58
1:B:156:LEU:O	1:B:160:ILE:HG13	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:215:TRP:CD1	1:B:216:ILE:N	2.71	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:267:MET:SD	1:C:267:MET:HE3	2.44	0.57
1:D:188:TYR:CD1	1:D:188:TYR:C	2.82	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:219:VAL:HG12	1:A:223:LEU:HD11	1.87	0.57
1:A:267:MET:HG2	1:B:271:ILE:HD13	1.86	0.56
1:B:215:TRP:NE1	1:B:216:ILE:CG1	2.67	0.56
1:C:270:LEU:HD13	1:C:270:LEU:H	1.70	0.56
1:D:215:TRP:HE1	1:D:216:ILE:HG13	1.62	0.56
1:D:221:PHE:CD1	1:D:221:PHE:C	2.82	0.56
1:B:215:TRP:CG	1:B:216:ILE:H	2.24	0.56
1:B:149:GLY:O	1:B:152:TRP:HB2	2.06	0.56
1:B:260:ALA:HA	1:B:263:GLU:HB3	1.86	0.56
1:A:268:LEU:HA	1:A:271:ILE:HD12	1.87	0.56
1:B:233:PHE:HZ	1:C:233:PHE:HE2	1.54	0.56
1:C:267:MET:HG3	1:D:268:LEU:HG	1.88	0.56
1:C:268:LEU:HD22	1:C:272:ARG:HH12	1.71	0.56
1:D:189:THR:O	1:D:193:VAL:N	2.35	0.56
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:C:225:SER:O	1:C:229:VAL:HG23	2.06	0.55
1:D:268:LEU:HD22	1:D:272:ARG:HH22	1.72	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:A:221:PHE:O	1:A:225:SER:CB	2.55	0.55
1:A:241:MET:HE1	1:B:241:MET:HB3	1.88	0.55
1:D:204:ALA:O	1:D:208:ILE:N	2.39	0.55
1:A:267:MET:CE	1:D:267:MET:SD	2.94	0.54
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:A:261:HIS:CE1	1:D:263:GLU:OE2	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLU:HG3	1:D:199:TRP:N	2.20	0.54
1:D:188:TYR:HE1	1:D:192:GLN:HG3	1.72	0.54
1:B:150:ILE:C	1:B:152:TRP:H	2.15	0.54
1:D:208:ILE:HA	1:D:214:ALA:HB3	1.89	0.54
1:C:177:PRO:CD	1:C:178:GLU:H	2.21	0.54
1:D:225:SER:O	1:D:229:VAL:HG23	2.07	0.54
1:A:179:TRP:HH2	1:A:206:PRO:HB2	1.71	0.54
1:B:199:TRP:CH2	1:B:200:SER:HB2	2.43	0.54
1:C:172:PHE:CD2	1:C:207:VAL:CG1	2.91	0.54
1:D:213:TRP:O	1:D:216:ILE:HB	2.08	0.54
1:C:266:GLU:O	1:C:270:LEU:HD13	2.08	0.54
1:A:215:TRP:CG	1:A:216:ILE:N	2.75	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: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:A:204:ALA:HB2	1:A:218:PHE:CG	2.43	0.53
1:B:229:VAL:O	1:B:232:LEU:N	2.40	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:C:274:LEU:C	1:C:276:SER:H	2.16	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:A:232:LEU:CD2	1:A:236:ILE:HD11	2.39	0.52
1:C:169:THR:O	1:C:173:ALA:CB	2.55	0.52
1:A:240:SER:HA	1:A:243:SER:OG	2.09	0.52
1:C:203:ILE:O	1:C:207:VAL:HG23	2.10	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:B:241:MET:CE	1:C:241:MET:HB3	2.40	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
1:A:200:SER:O	1:A:205:ARG:CG	2.58	0.52
1:A:271:ILE:HG21	1:D:270:LEU:HB3	1.91	0.52
1:D:188:TYR:O	1:D:192:GLN:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:SER:O	1:D:221:PHE:C	2.51	0.52
1:A:160:ILE:HA	1:A:163:VAL:HG22	1.91	0.52
1:A:172:PHE:HB3	1:A:176:PHE:HD2	1.75	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:D:233:PHE:CE2	1:D:237:ILE:HD11	2.45	0.51
1:A:241:MET:SD	1:D:241:MET:HE1	2.51	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:A:204:ALA:CB	1:A:218:PHE:CD1	2.93	0.51
1:D:215:TRP:CE2	1:D:216:ILE:CG1	2.79	0.51
1:D:194:MET:HE2	1:D:194:MET:O	2.10	0.51
1:D:208:ILE:HG22	1:D:209:GLU:N	2.24	0.51
1:C:241:MET:HE1	1:D:241:MET:HB3	1.91	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:D:150:ILE:C	1:D:152:TRP:N	2.65	0.51
1:B:155:LEU:O	1:B:159:VAL:N	2.41	0.50
1:A:157:LEU:O	1:A:160:ILE:HB	2.11	0.50
1:A:220:SER:HA	1:A:223:LEU:HD12	1.92	0.50
1:D:188:TYR:C	1:D:188:TYR:HD1	2.19	0.50
1:B:150:ILE:C	1:B:152:TRP:N	2.69	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:D:220:SER:HA	1:D:223:LEU:HD12	1.93	0.49
1:A:152:TRP:HA	1:A:152:TRP:CE3	2.47	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:C:215:TRP:CG	1:C:216:ILE:N	2.80	0.49
1:A:192:GLN:HG3	1:B:200:SER:HB3	1.93	0.49
1:D:215:TRP:CG	1:D:216:ILE:H	2.26	0.49
1:A:221:PHE:O	1:A:225:SER:HB3	2.13	0.48
1:C:175:SER:C	1:C:177:PRO:HD3	2.38	0.48
1:D:260:ALA:C	1:D:262:ASP:N	2.70	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:179:TRP:HZ3	1:C:207:VAL:CG2	2.20	0.48
1:C:197:GLU:HG3	1:D:199:TRP:CD1	2.48	0.48
1:C:197:GLU:OE1	1:D:201:MET:HB2	2.13	0.48
1:C:267:MET:HB2	1:D:268:LEU:HD21	1.95	0.48
1:C:269:GLN:HE22	1:C:273:ASP:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:TYR:O	1:C:189:THR:C	2.57	0.48
1:D:173:ALA:HA	1:D:180:PHE:C	2.39	0.48
1:B:208:ILE:HD11	1:B:215:TRP:CA	2.42	0.48
1:C:268:LEU:O	1:C:271:ILE:HB	2.14	0.48
1:B:229:VAL:O	1:B:230:LEU:C	2.57	0.47
1:B:154:ALA:O	1:B:158:LEU:N	2.46	0.47
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:D:229:VAL:O	1:D:233:PHE:N	2.34	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: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: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:215:TRP:NE1	1:A:216:ILE:CG1	2.74	0.47
1:B:156:LEU:O	1:B:159:VAL:HB	2.15	0.47
1:D:191:PHE:HA	1:D:194:MET:CB	2.43	0.46
1:B:194:MET:O	1:B:194:MET:HE2	2.15	0.46
1:C:160:ILE:HD11	1:C:228:THR:HG21	1.98	0.46
1:D:211:TYR:O	1:D:214:ALA:CB	2.63	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:B:202:GLY:O	1:B:206:PRO:HG2	2.16	0.46
1:D:264:ARG:HA	1:D:267:MET:HB3	1.98	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:A:175:SER:C	1:A:177:PRO:HD3	2.41	0.45
1:A:259:ARG:HA	1:A:262:ASP:HB2	1.97	0.45
1:B:153:ILE:O	1:B:157:LEU:HB3	2.17	0.45
1:D:202:GLY:C	1:D:203:ILE:HD13	2.41	0.45
1:B:161:PHE:O	1:B:162:TYR:C	2.59	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:H	1:B:153:ILE:HG13	1.49	0.45
1:B:234:ILE:HG13	1:B:237:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:GLN:C	1:C:269:GLN:CD	2.85	0.45
1:A:159:VAL:O	1:A:163:VAL:HG13	2.17	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
1:D:200:SER:HA	1:D:204:ALA:HB3	1.98	0.45
1:A:193:VAL:O	1:A:196:LEU:HD23	2.17	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: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:HB2	1:A:180:PHE:HB2	1.98	0.44
1:A:172:PHE:CB	1:A:180:PHE:CD2	2.99	0.44
1:D:203:ILE:O	1:D:207:VAL:HG23	2.16	0.44
1:A:197:GLU:OE2	1:B:200:SER:HB3	2.18	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:241:MET:HB2	1:D:241:MET:HE3	2.00	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:D:264:ARG:O	1:D:265:LEU:C	2.60	0.44
1:A:237:ILE:O	1:A:241:MET:CB	2.58	0.44
1:D:161:PHE:CZ	1:D:191:PHE:HB2	2.52	0.44
1:D:234:ILE:HG13	1:D:237:ILE:HD12	1.99	0.44
1:D:276:SER:O	1:D:280:ARG:N	2.43	0.44
1:C:153:ILE:HG23	1:C:156:LEU:CD2	2.48	0.43
1:D:269:GLN:HA	1:D:269:GLN:NE2	2.30	0.43
1:D:164:PHE:HD1	1:D:164:PHE:HA	1.68	0.43
1:C:274:LEU:C	1:C:276:SER:N	2.77	0.43
1:A:207:VAL:HG11	1:A:218:PHE:HZ	1.81	0.43
1:C:266:GLU:CD	1:C:267:MET:N	2.76	0.43
1:D:171:LEU:N	1:D:171:LEU:CD1	2.81	0.43
1:D:196:LEU:HA	1:D:199:TRP:HB3	2.00	0.43
1:B:215:TRP:HE1	1:B:216:ILE:CD1	2.32	0.43
1:D:162:TYR:CD1	1:D:162:TYR:C	2.97	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:B:221:PHE:O	1:B:225:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:PHE:CD1	1:C:172:PHE:N	2.86	0.43
1:A:183:LEU:C	1:A:185:ALA:H	2.27	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:C:192:GLN:O	1:C:195:THR:OG1	2.36	0.43
1:B:151:ALA:O	1:B:154:ALA:HB3	2.19	0.42
1:B:203:ILE:O	1:B:207:VAL:CG2	2.62	0.42
1:B:281:LEU:C	1:B:283:ARG:N	2.75	0.42
1:C:274:LEU:HD21	1:D:274:LEU:HG	2.01	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:A:180:PHE:HD1	1:A:186:SER:OG	2.02	0.42
1:A:237:ILE:HG22	1:A:241:MET:HG3	2.00	0.42
1:A:161:PHE:HZ	1:A:191:PHE:HA	1.84	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:D:215:TRP:CE3	1:D:219:VAL:HG21	2.55	0.42
1:A:149:GLY:H	1:A:152:TRP:HB2	1.85	0.42
1:A:171:LEU:CD2	1:A:213:TRP:CZ2	3.02	0.42
1:A:275:SER:OG	1:D:274:LEU:HD13	2.20	0.42
1:B:191:PHE:HE2	1:C:199:TRP:CZ2	2.38	0.42
1:D:211:TYR:O	1:D:214:ALA:HB2	2.20	0.42
1:A:205:ARG:HE	1:D:192:GLN:HE21	1.66	0.42
1:B:234:ILE:HA	1:B:237:ILE:HD12	2.00	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:B:208:ILE:C	1:B:210:ALA:N	2.76	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:A:222:ILE:O	1:A:226:SER:N	2.51	0.41
1:C:263:GLU:OE2	1:D:261:HIS:CG	2.72	0.41
1:D:153:ILE:HD11	1:D:232:LEU:HG	2.02	0.41
1:A:237:ILE:H	1:A:237:ILE:HG13	1.68	0.41
1:D:173:ALA:HA	1:D:180:PHE:O	2.21	0.41
1:D:265:LEU:O	1:D:269:GLN:HG2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLY:HA2	1:A:172:PHE:HD2	1.86	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:D:183:LEU:O	1:D:186:SER:HB2	2.20	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:B:161:PHE:HD1	1:B:161:PHE:HA	1.81	0.41
1:C:163:VAL:HG12	1:C:164:PHE:N	2.36	0.41
1:C:193:VAL:O	1:C:194:MET:C	2.62	0.41
1:A:164:PHE:CE2	1:A:221:PHE:HA	2.56	0.41
1:A:168:GLY:HA2	1:A:172:PHE:CD2	2.56	0.41
1:A:176:PHE:CE2	1:A:210:ALA:HB3	2.54	0.41
1:A:179:TRP:CZ3	1:A:203:ILE:O	2.74	0.41
1:C:208:ILE:O	1:C:212:PRO:HA	2.20	0.41
1:C:234:ILE:HA	1:C:237:ILE:HD12	2.02	0.41
1:D:190:LEU:HD23	1:D:190:LEU:HA	1.68	0.41
1:A:194:MET:HG2	1:A:225:SER:OG	2.21	0.40
1:A:277:LYS:O	1:A:278:VAL:C	2.62	0.40
1:B:151:ALA:HA	1:B:154:ALA:HB3	2.02	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: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:C:157:LEU:O	1:C:160:ILE:HB	2.21	0.40
1:D:153:ILE:CD1	1:D:232:LEU:HG	2.51	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	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
All	All	544/608 (90%)	469 (86%)	75 (14%)	0	100	100

There are no Ramachandran outliers to report.

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	96/131 (73%)	73 (76%)	23 (24%)	1	4
1	B	95/131 (72%)	79 (83%)	16 (17%)	2	13
1	C	93/131 (71%)	75 (81%)	18 (19%)	1	8
1	D	91/131 (70%)	68 (75%)	23 (25%)	0	3
All	All	375/524 (72%)	295 (79%)	80 (21%)	1	6

All (80) 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	164	PHE
1	A	166	VAL
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	203	ILE

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Mol	Chain	Res	Type
1	A	223	LEU
1	A	229	VAL
1	A	237	ILE
1	A	241	MET
1	A	255	GLU
1	A	262	ASP
1	A	266	GLU
1	A	268	LEU
1	A	278	VAL
1	A	279	ASP
1	B	153	ILE
1	B	155	LEU
1	B	156	LEU
1	B	157	LEU
1	B	158	LEU
1	B	161	PHE
1	B	163	VAL
1	B	174	GLN
1	B	182	THR
1	B	194	MET
1	B	196	LEU
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	164	PHE
1	C	180	PHE
1	C	182	THR
1	C	183	LEU
1	C	194	MET
1	C	232	LEU
1	C	234	ILE
1	C	236	ILE
1	C	240	SER
1	C	241	MET
1	C	255	GLU
1	C	268	LEU
1	C	270	LEU

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Mol	Chain	Res	Type
1	C	275	SER
1	C	282	GLU
1	D	152	TRP
1	D	155	LEU
1	D	157	LEU
1	D	158	LEU
1	D	159	VAL
1	D	163	VAL
1	D	164	PHE
1	D	171	LEU
1	D	174	GLN
1	D	182	THR
1	D	183	LEU
1	D	190	LEU
1	D	192	GLN
1	D	194	MET
1	D	200	SER
1	D	201	MET
1	D	208	ILE
1	D	228	THR
1	D	236	ILE
1	D	238	ILE
1	D	240	SER
1	D	266	GLU
1	D	272	ARG

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

Mol	Chain	Res	Type
1	A	192	GLN
1	A	261	HIS
1	C	192	GLN
1	C	269	GLN
1	D	192	GLN
1	D	231	ASN
1	D	269	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	138/152 (90%)	-0.53	1 (0%) 84 64	54, 193, 260, 400	0
1	B	138/152 (90%)	-0.73	0 100 100	130, 195, 276, 313	0
1	C	138/152 (90%)	-0.81	0 100 100	112, 185, 246, 349	0
1	D	138/152 (90%)	-0.76	0 100 100	114, 178, 249, 317	0
All	All	552/608 (90%)	-0.71	1 (0%) 91 83	54, 188, 265, 400	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	TRP	7.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	CA	A	301	1/1	0.88	0.13	212,212,212,212	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	303	1/1	0.92	0.08	234,234,234,234	0
2	CA	D	301	1/1	0.92	0.04	178,178,178,178	0
3	NI	A	303	1/1	0.97	0.23	146,146,146,146	0
2	CA	B	301	1/1	0.99	0.11	113,113,113,113	0
2	CA	A	302	1/1	0.99	0.09	180,180,180,180	0
2	CA	B	302	1/1	1.00	0.03	145,145,145,145	0

6.5 Other polymers [i](#)

There are no such residues in this entry.